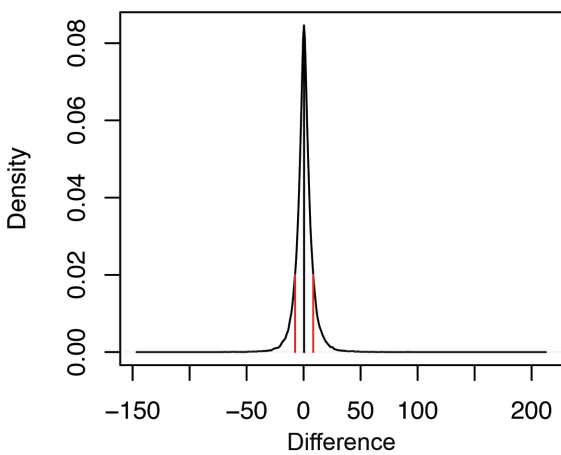


SUPPLEMENTARY DATA

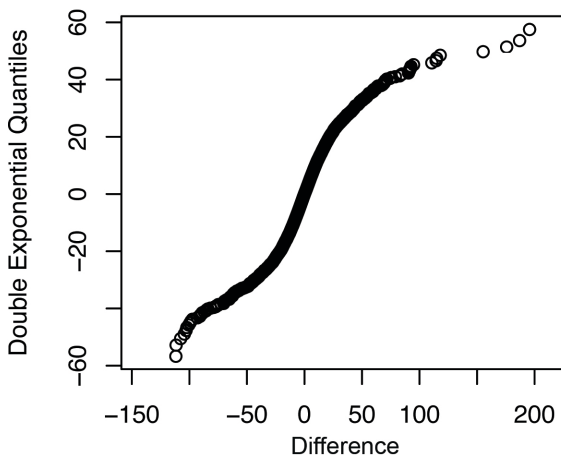
Supplementary Figure 1. Identification and elimination of statistical outliers. **(a)** Kernel density plot of difference (D) from duplicate observations for each kinase-inhibitor pair. The estimated double exponential density (y-axis) is plotted against D (x-axis). The grey vertical lines represent one standard deviation on either side of the mean of the distribution of D. **(b)** Quantile-quantile plot of D from duplicate observations for each kinase-inhibitor pair. Quantiles of the estimated double exponential distribution (y-axis) are plotted against D (x-axis). **(c)** Kernel density plot of the coefficient of variation (CV) from duplicate observations for each kinase-inhibitor pair. The estimated log-normal density (y-axis) is plotted against CV (x-axis). **(d)** Quantile-quantile plot of CV from duplicate observations for each kinase-inhibitor pair. Quantiles of the estimated log-normal distribution (y-axis) are plotted against CV (x-axis). **(e)** A scatter plot of CV versus D for all kinase-inhibitor pairs. The green and black circles that lie inside the band formed by the red vertical lines represent observations within one standard deviation of the mean of the estimated double exponential distribution of D. These observations were considered to be within acceptable noise levels in assay measurements and were retained for further analyses of compound activity. The pink horizontal line represents the CV threshold for outlier detection. The blue circles represent observations whose CV exceeded this threshold and were identified as outliers. **(f)** A scatter plot of the kinase activity in replicate 1 versus replicate 2 for all kinase-inhibitor pairs. Data points in black represent the identified outliers that were removed from the final data.

Supplementary Figure 1

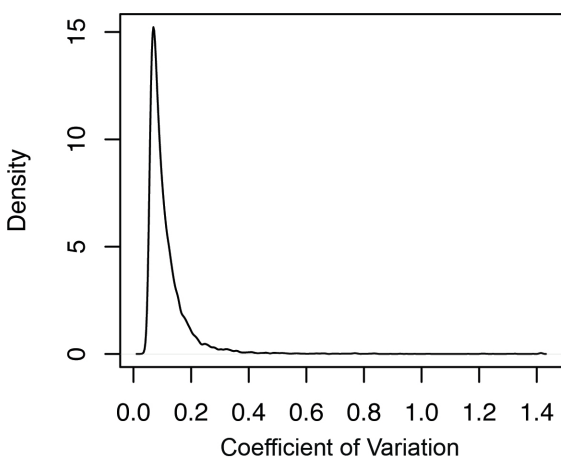
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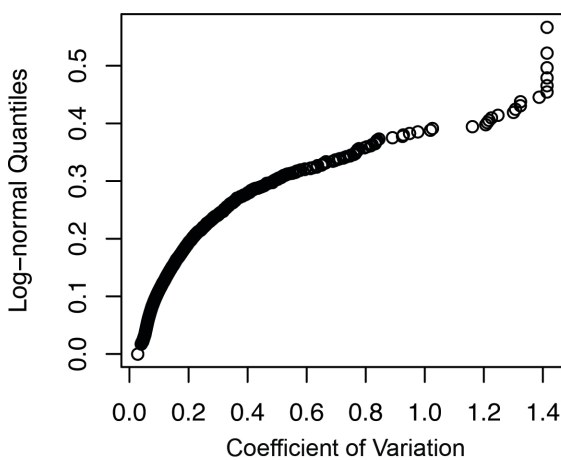
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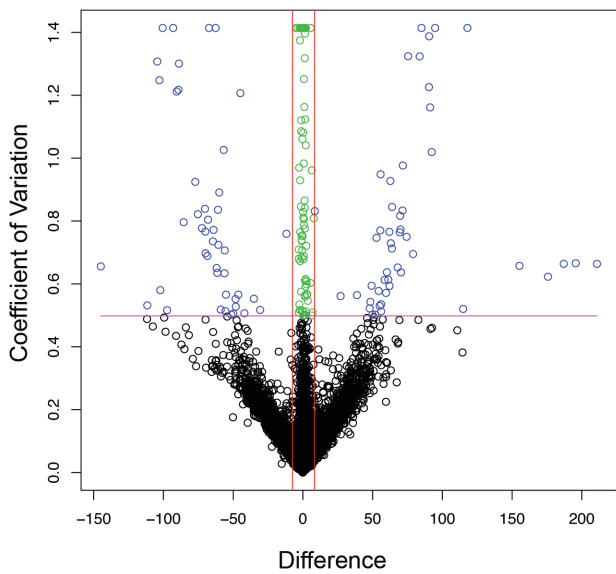
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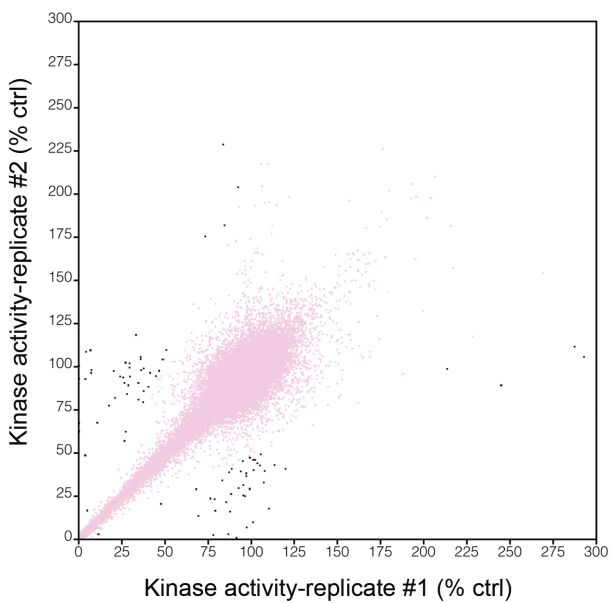
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e



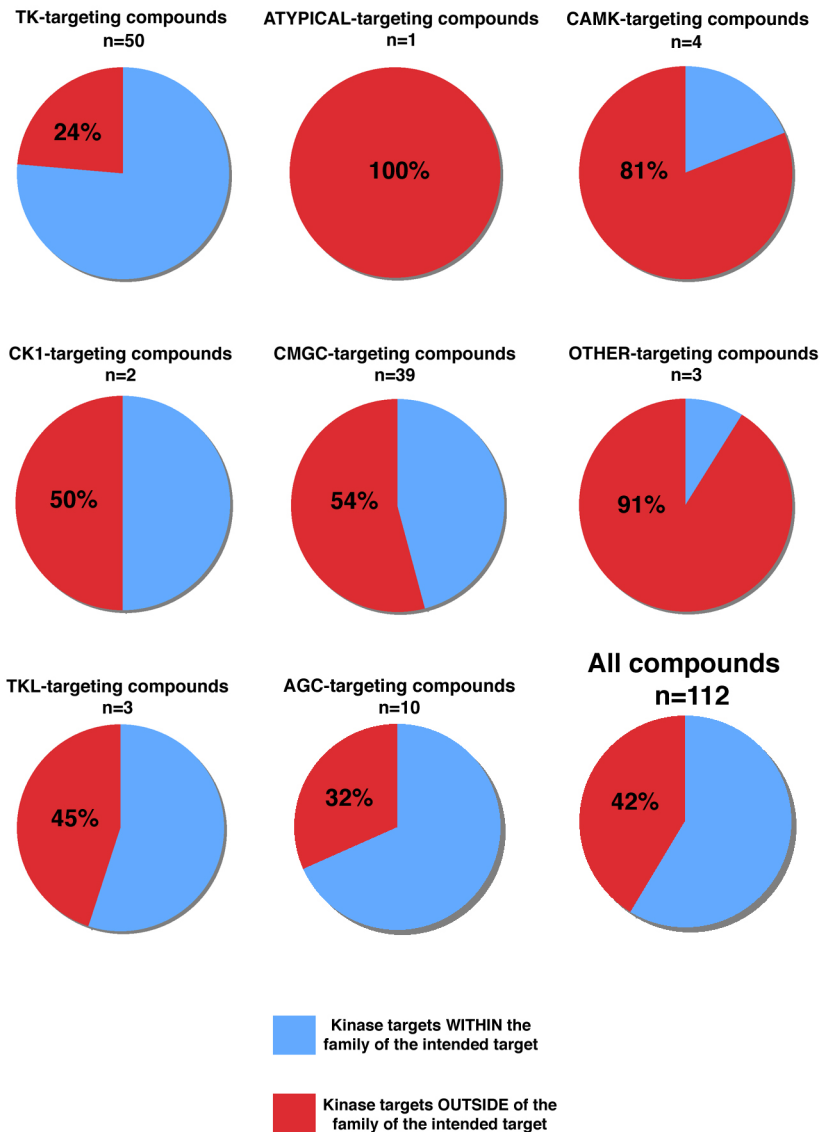
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Supplementary Figure 2. A high-resolution version of **Figure 1d** showing two-way hierarchical clustering analysis of the entire kinase-inhibitor interaction network presented as a heatmap of inhibitory activity.

Supplementary Figure 3. Kinase inhibitors frequently inhibit kinases outside of the subfamily containing their intended targets. All compounds intended to target a kinase in the indicated specific subfamily of kinases were analyzed as to whether the kinases they inhibit fall within the subfamily of their intended target (blue) or outside of that family (red, percent of total shown). The final pie chart presents aggregate data for all of the subfamilies presented. “n” reports the number of compounds analyzed for each target subfamily. The following compound types were not included in this analysis: compounds intended to target lipid kinases, inactive control compounds, compounds intended to target kinases from multiple subfamilies, compounds that did not inhibit any kinases. For example, none of the four compounds intended to target STE subfamily kinases inhibited any kinases significantly.

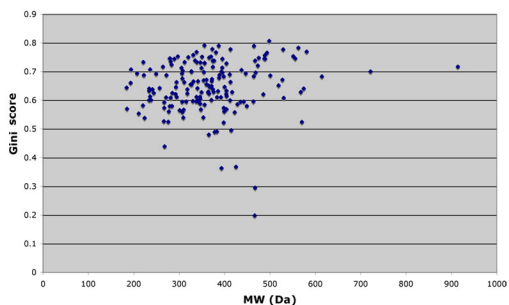
Supplementary Figure 3



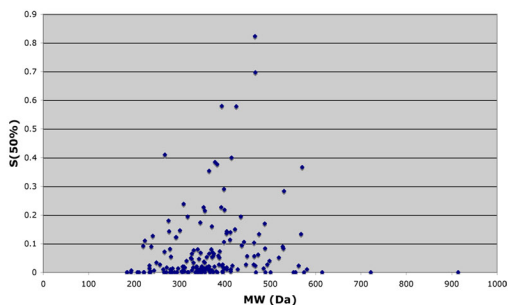
Supplementary Figure 4. No single physicochemical property correlates with inhibitor selectivity. All 178 test compounds were analyzed with regard to molecular weight, predicted LogP, polar surface area (PSA), number of hydrogen bond acceptors, and number of hydrogen bond donors. These features are plotted for each compound as a function of inhibitor selectivity from the screening data reported either as Gini score (from Supplementary Table 5) or as Selectivity score ($S_{(50\%)}$). The Selectivity score of a compound corresponds to the number of kinases that it inhibited by at least 50% divided by the number of kinases against which the compound was tested. More selective inhibitors are associated with lower Selectivity scores and higher Gini scores.

Supplementary Figure 4

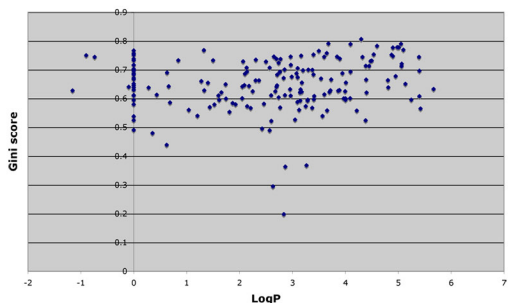
Molecular Weight vs Gini score



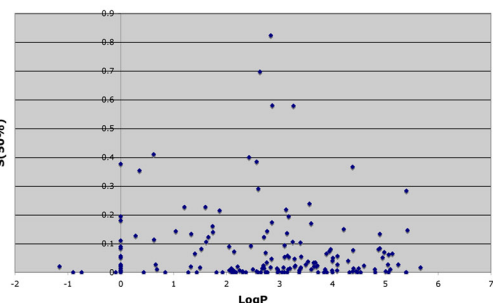
Molecular Weight vs Selectivity score



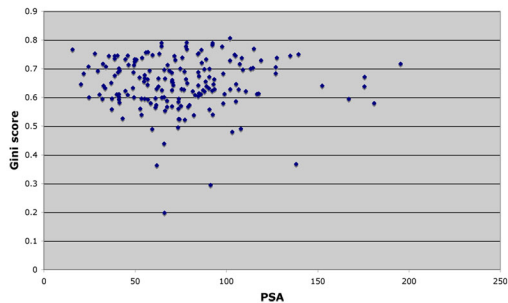
LogP vs Gini score



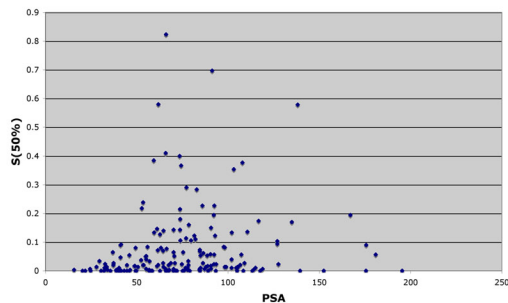
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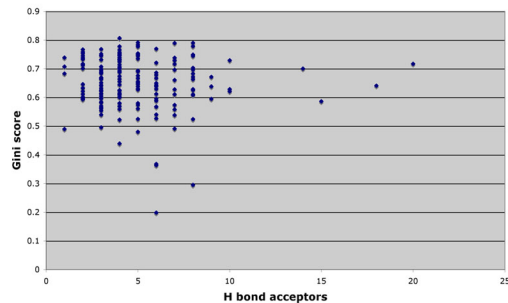
Polar surface area vs Gini score



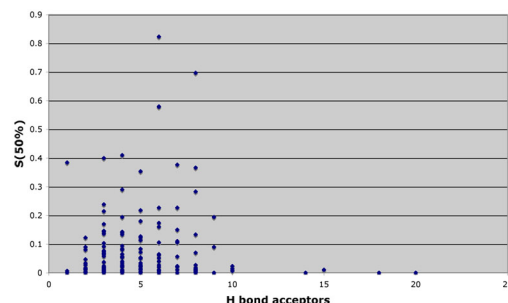
Polar surface area vs Selectivity score



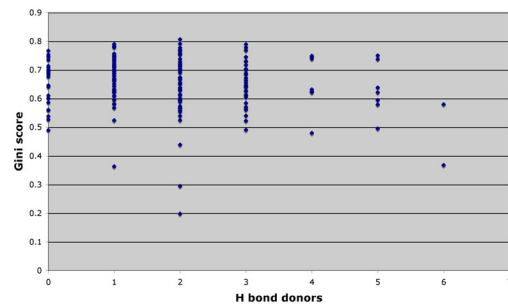
H bond acceptor vs Gini score



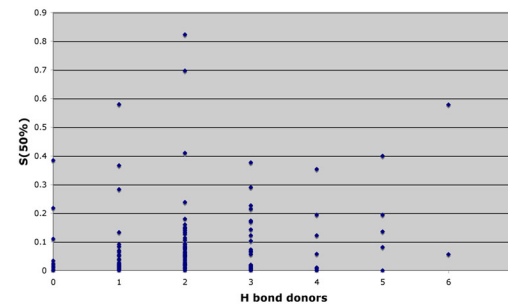
H bond acceptor vs Selectivity score



H bond donor vs Gini score



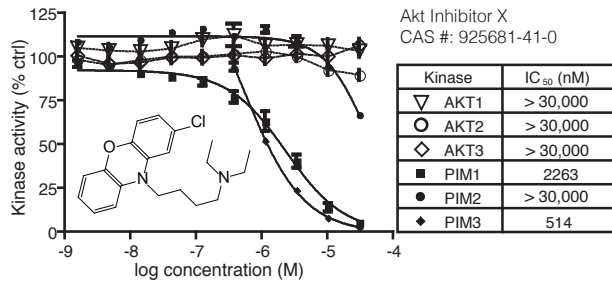
H bond donor vs Selectivity score



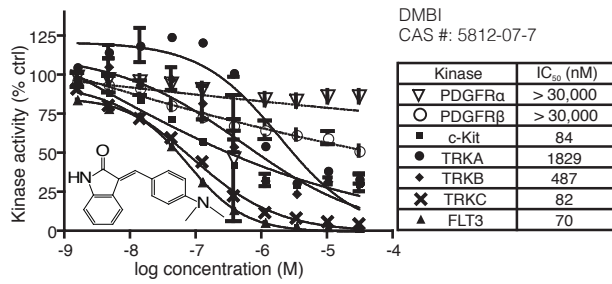
Supplementary Figure 5. Validation of novel uni-specific kinase inhibitors. Complete *in vitro* kinase assay dose-response results are shown for the five indicated uni-specific compounds (**a-e**) from **Figure 5** against both the intended targets of each inhibitor and their novel, more potently inhibited target(s). Data for intended kinase target(s) are shown with open symbols and novel target(s) with closed symbols. Data points represent averages of two independent replicates. Error bars denote standard error of the mean. Data exhibiting significant inhibition was fitted with a sigmoidal dose-response curve to derive IC₅₀ values.

Supplementary Figure 5

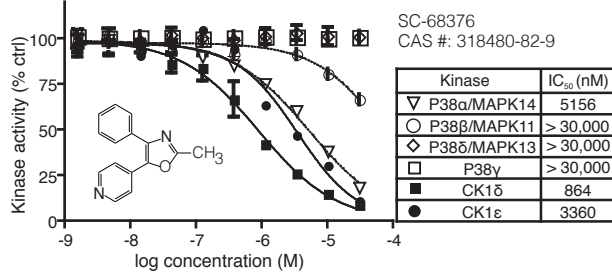
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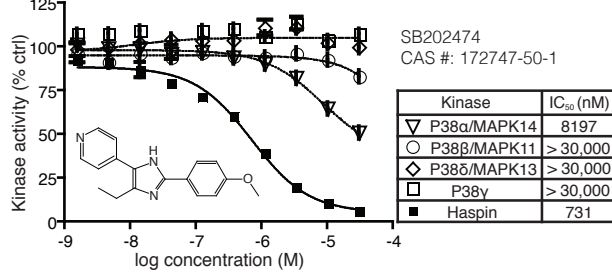
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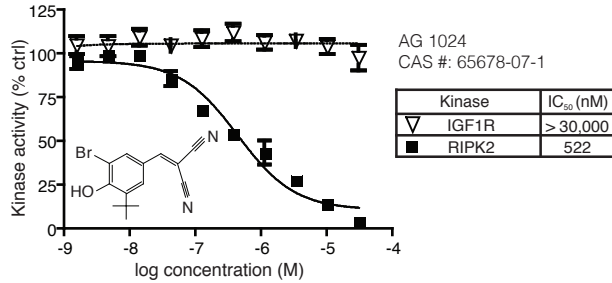
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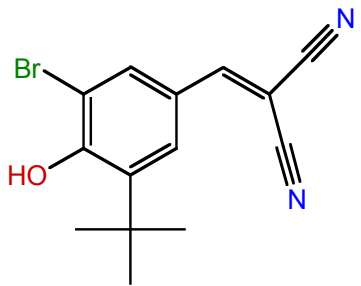
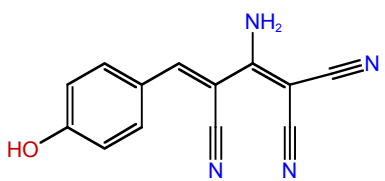
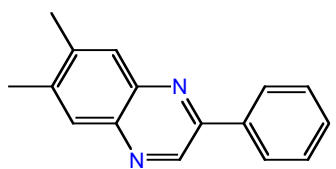
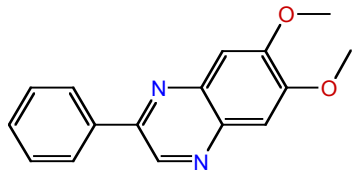
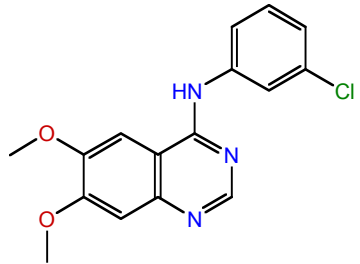
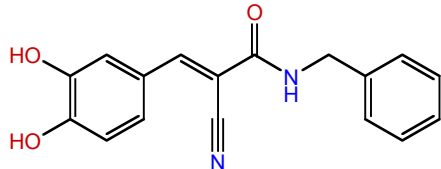
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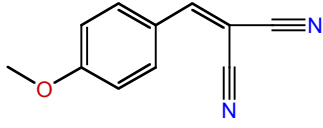
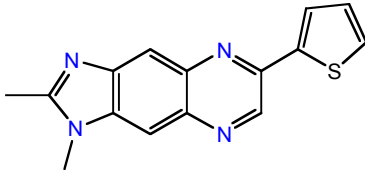
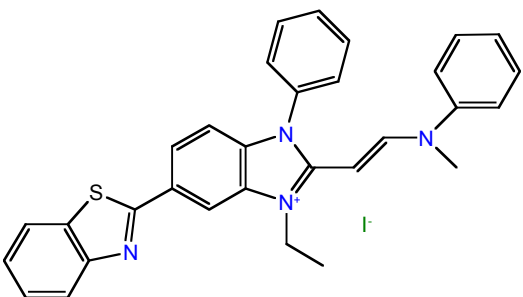
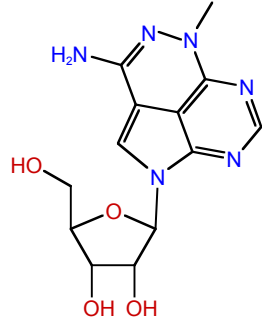
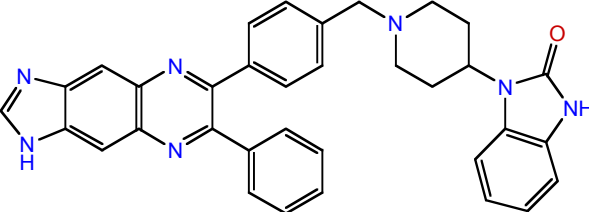


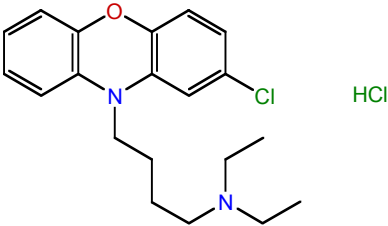
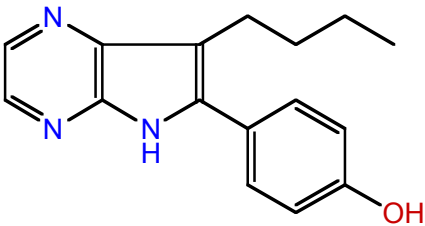
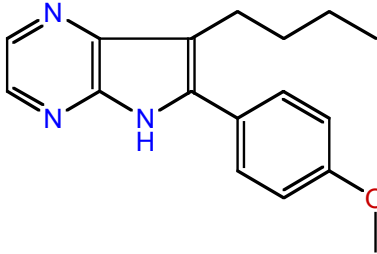
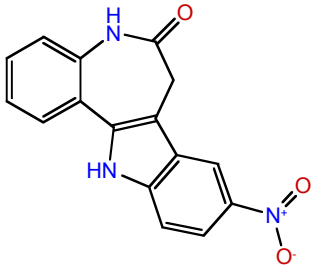
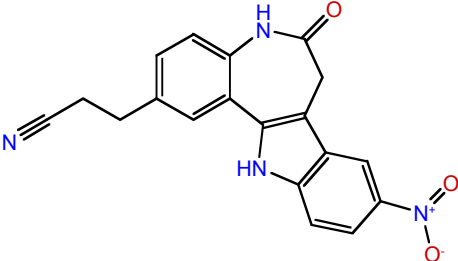
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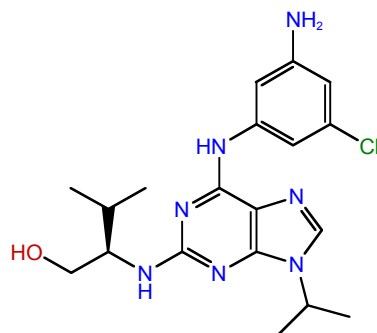
Supplementary Table 1. Compounds used in this study.

Name	CAS #	Structure	Target family
AG 1024	65678-07-1		TK
AG 112	144978-82-5		TK
AG 1295	71897-07-9		TK
AG 1296	146535-11-7		TK
AG 1478	175178-82-2		TK
AG 490	133550-30-8		TK

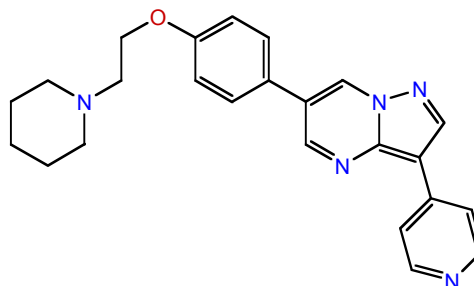
AG 9	2826-26-8		TK
AGL 2043	226717-28-8		TK
Akt Inhibitor IV	681281-88-9		AGC
Akt Inhibitor V, Triciribine	35943-35-2		AGC
Akt Inhibitor VIII, Isozyme-Selective, Akti-1/2	612847-09-3		AGC

Akt Inhibitor X	925681-41-0		AGC
Aloisine A, RP107	496864-16-5		CMGC
Aloisine, RP106	496864-15-4		CMGC
Alsterpaullone	237430-03-4		CMGC
Alsterpaullone, 2-Cyanoethyl	852527-97-0		CMGC

Aminopurvalanol A 220792-57-4

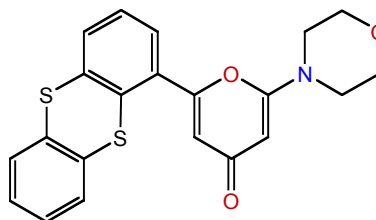


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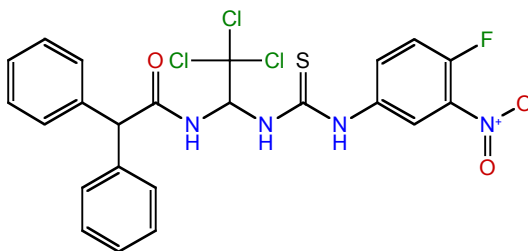
AMPK Inhibitor,
Compound C 866405-64-3

CAMK

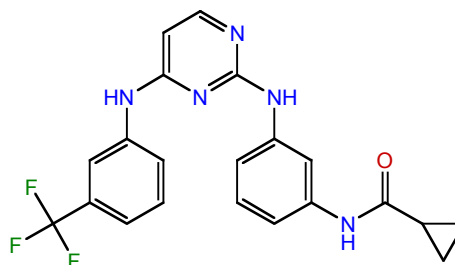
ATM Kinase Inhibitor 587871-26-9



ATYPICAL

ATM/ATR Kinase
Inhibitor 905973-89-9

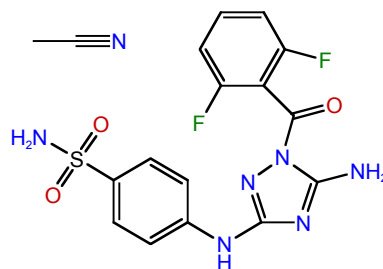
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Aurora Kinase
Inhibitor III 879127-16-9

OTHER

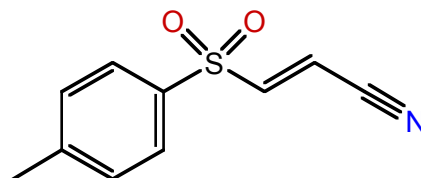
Aurora Kinase/
Cdk Inhibitor

443797-96-4

OTHER,
CMGC

BAY 11-7082

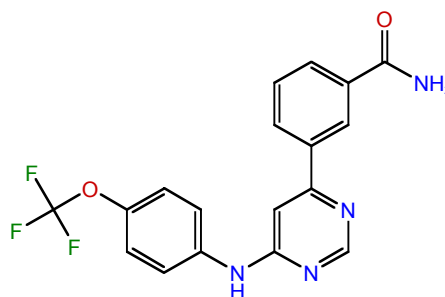
19542-67-7



OTHER

Bcr-abl Inhibitor

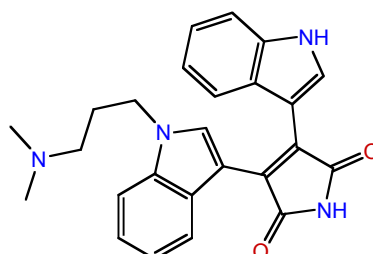
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TK

Bisindolylmaleimide I

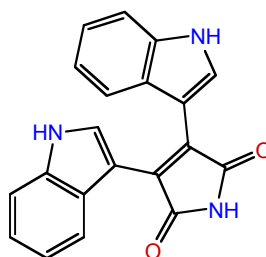
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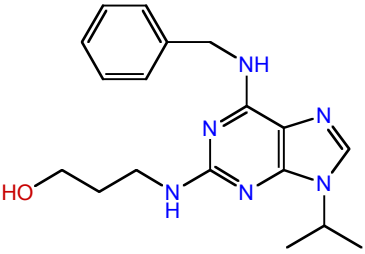
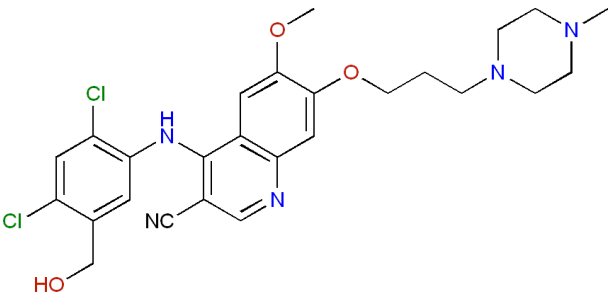
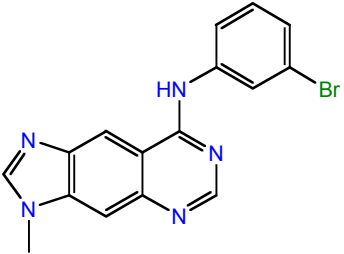
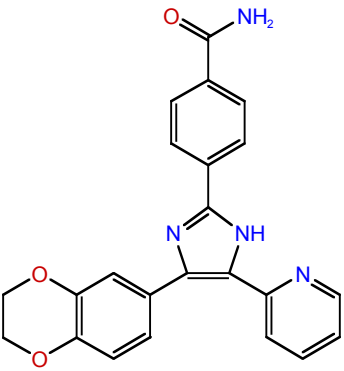
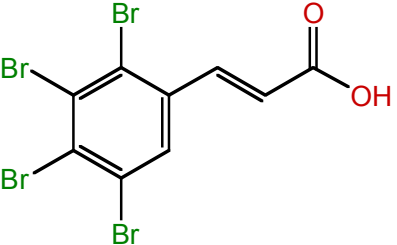
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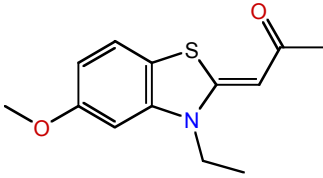
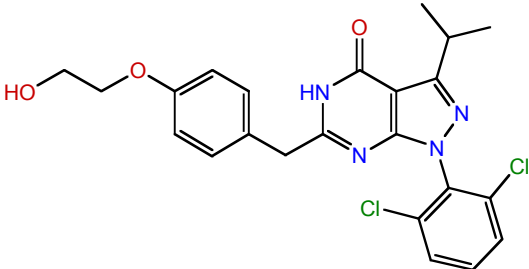
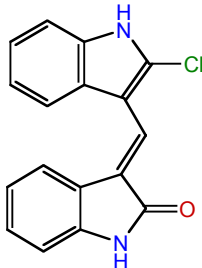
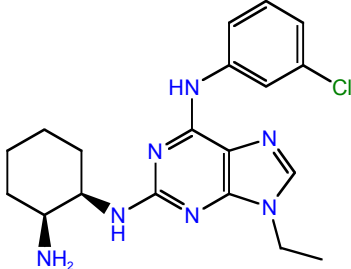
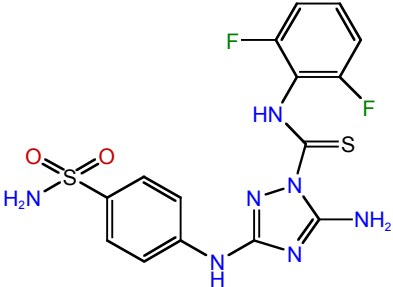
Bisindolylmaleimide IV

119139-23-0



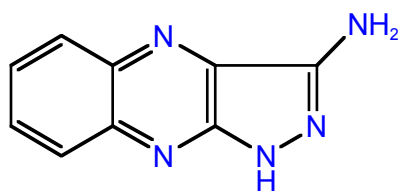
AGC

Bohemine	189232-42-6		CMGC
Bosutinib	380843-75-4		TK
BPIQ-I	174709-30-9		TK
Casein Kinase I Inhibitor, D4476	301836-43-1		CK1, CMGC, TKL
Casein Kinase II Inhibitor III, TBCA	934358-00-6		CK1

Cdc2-Like Kinase Inhibitor, TG003	300801-52-9		CMGC
Cdk/Crk Inhibitor	784211-09-2		CMGC
Cdk1 Inhibitor	220749-41-7		CMGC
Cdk1 Inhibitor, CGP74514A	190654-01-4		CMGC
Cdk1/2 Inhibitor III	443798-55-8		CMGC

Cdk1/5 Inhibitor

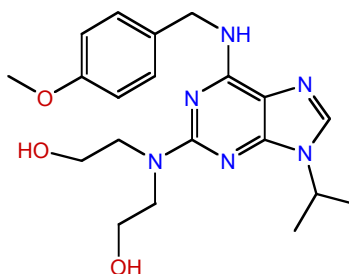
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CMGC

Cdk2 Inhibitor III

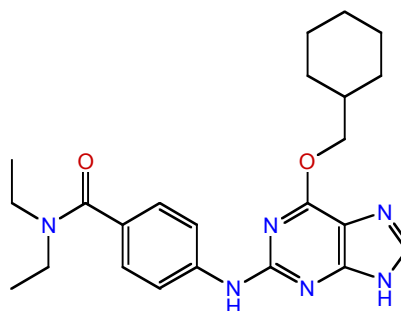
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CMGC

Cdk2 Inhibitor IV,
NU6140

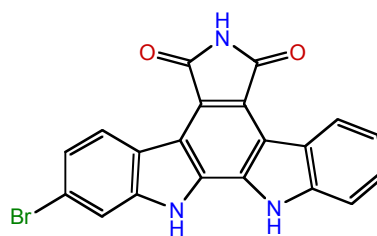
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CMGC

Cdk4 Inhibitor

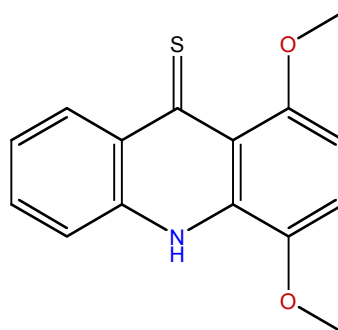
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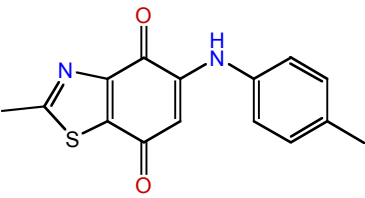
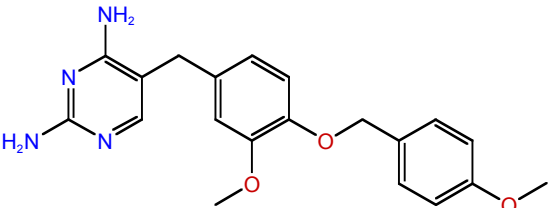
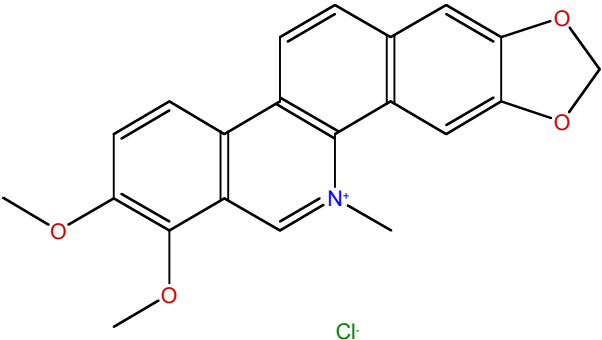
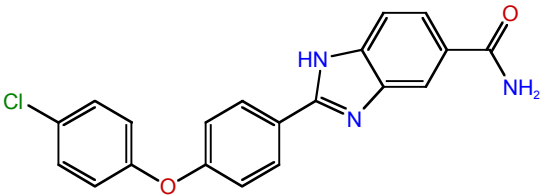
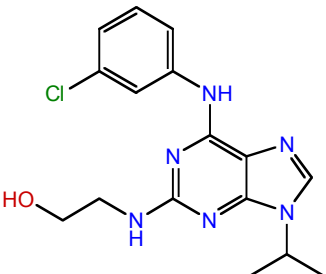
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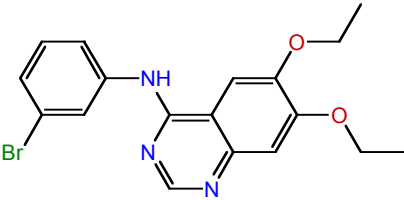
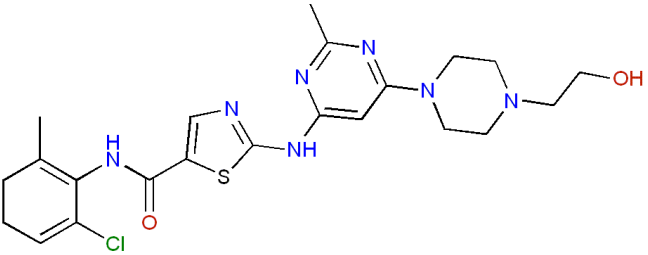
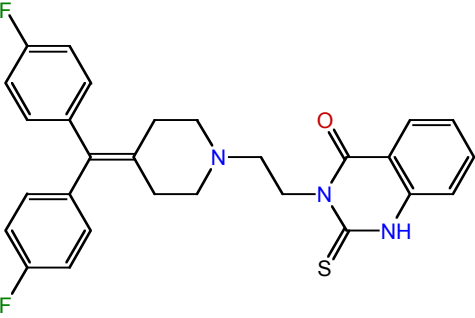
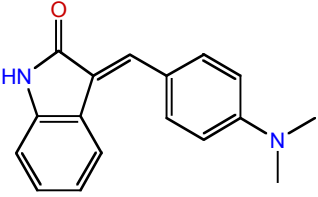
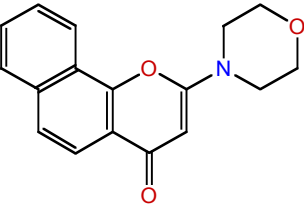
Cdk4 Inhibitor II,
NSC 625987

141992-47-4

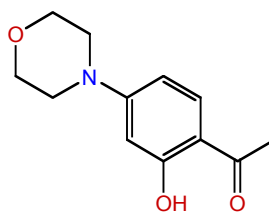


CMGC

Cdk4 Inhibitor III	265312-55-8		CMGC
cFMS Receptor Tyrosine Kinase Inhibitor	870483-87-7		TK
Chelerythrine Chloride	3895-92-9		AGC
Chk2 Inhibitor II	516480-79-8		CAMK
Compound 52	212779-48-1		CMGC

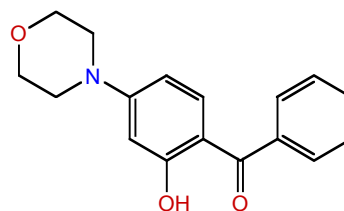
Compound 56	171745-13-4		TK
Dasatinib	302962-49-8		TK
Diacylglycerol Kinase Inhibitor II	120166-69-0		LIPID
DMBI	5812-07-7		TK
DNA-PK Inhibitor II	154447-35-5		ATYPICAL

DNA-PK Inhibitor III 404009-40-1



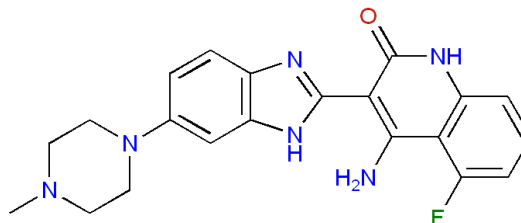
ATYPICAL

DNA-PK Inhibitor V 404009-46-7



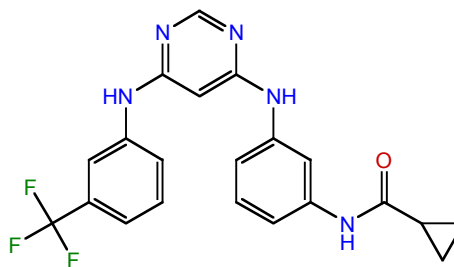
ATYPICAL

Dovitinib 405169-16-6



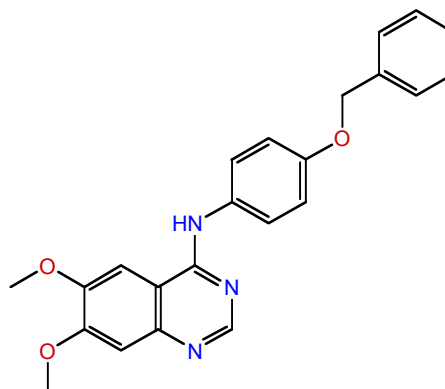
TK

EGFR Inhibitor 879127-07-8

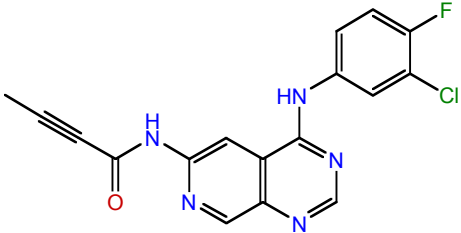
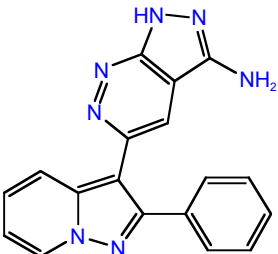
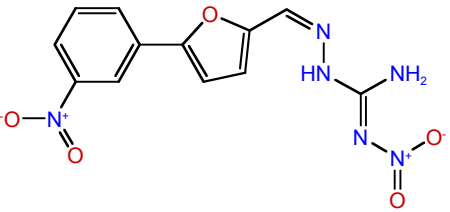
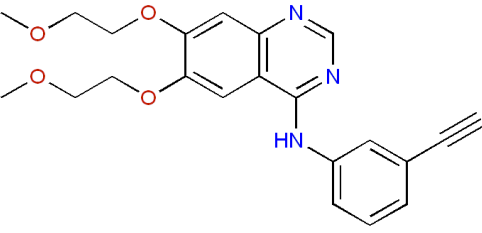
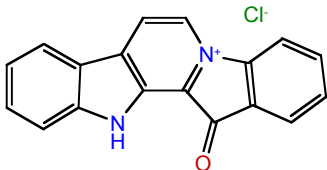


TK

EGFR/ErbB-2 Inhibitor 179248-61-4

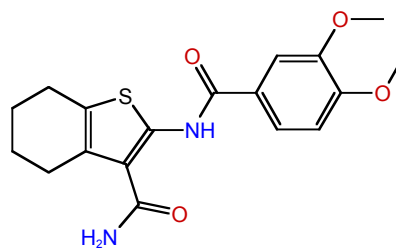


TK

EGFR/ErbB-2/ErbB-4 Inhibitor	881001-19-0		TK
ERK Inhibitor II, FR180204	865362-74-9		CMGC
ERK Inhibitor III	345616-52-6		CMGC
Erlotinib	183319-69-9		TK
Fascaplysin, Synthetic	114719-57-2		CMGC

Flt-3 Inhibitor

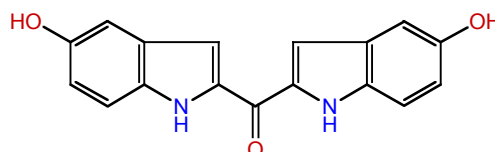
301305-73-7



TK

Flt-3 Inhibitor II

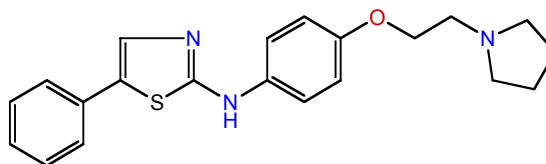
896138-40-2



TK

Flt-3 Inhibitor III

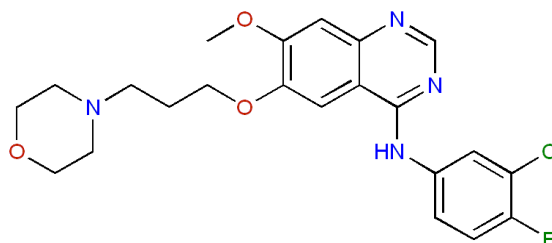
852045-46-6



TK

Gefitinib

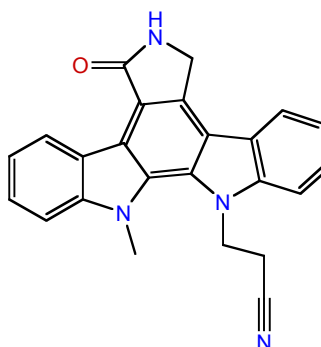
184475-35-2



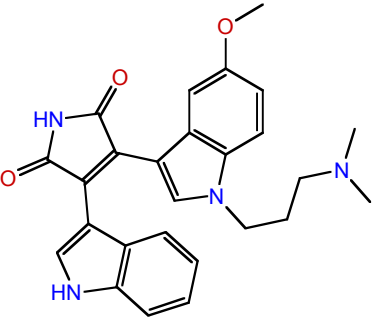
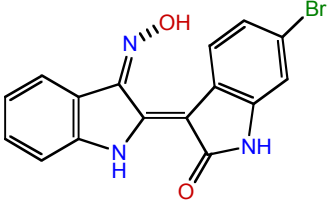
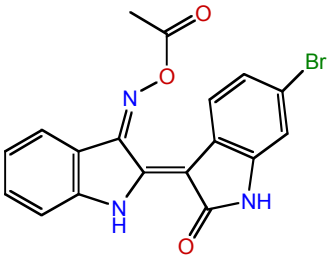
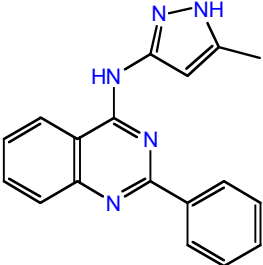
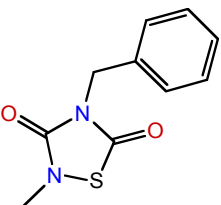
TK

Gö 6976

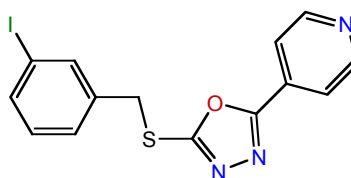
136194-77-9



AGC

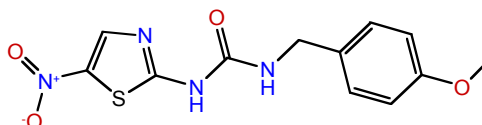
Gö 6983	133053-19-7		AGC
GSK-3 Inhibitor IX	667463-62-9		CMGC
GSK-3 Inhibitor X	740841-15-0		CMGC
GSK-3 Inhibitor XIII	404828-08-6		CMGC
GSK-3b Inhibitor I	327036-89-5		CMGC, AGC, TK

GSK-3b Inhibitor II 478482-75-6



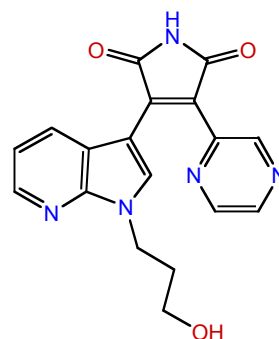
CMGC

GSK-3b Inhibitor VIII 487021-52-3

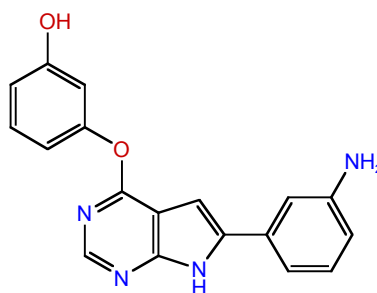


CMGC

GSK-3b Inhibitor XI 626604-39-5

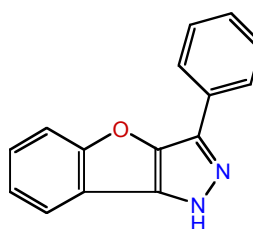


CMGC

GSK3b Inhibitor XII,
TWS119 601514-19-6

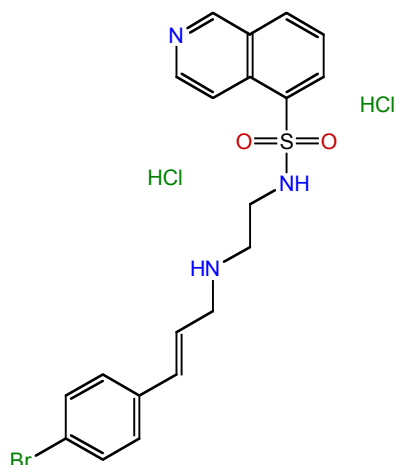
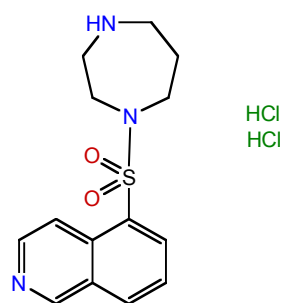
CMGC

GTP-14564 34823-86-4

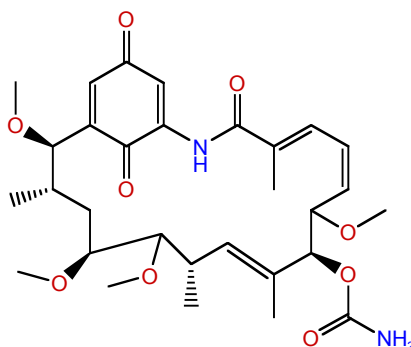


TK

H-89, Dihydrochloride 127243-85-0

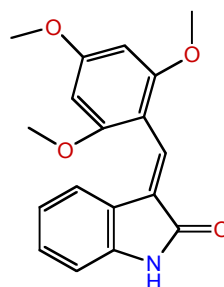
AGC, CK1,
CAMKHA 1077,
Dihydrochloride
Fasudil 103745-39-7

AGC

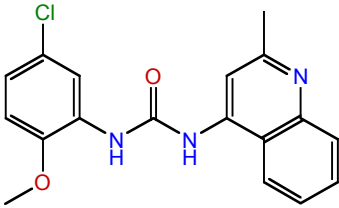
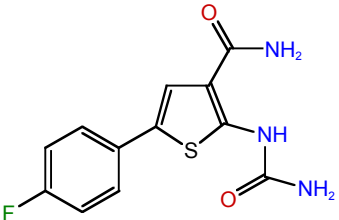
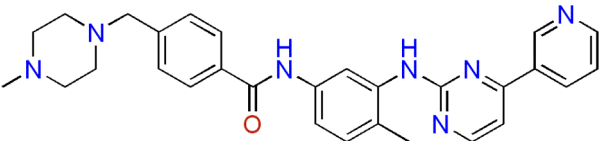
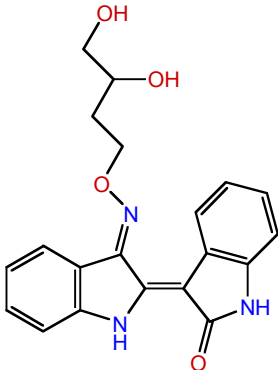
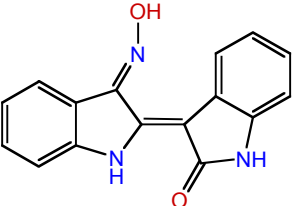
Herbimycin A,
Streptomyces sp. 70563-58-5

TK

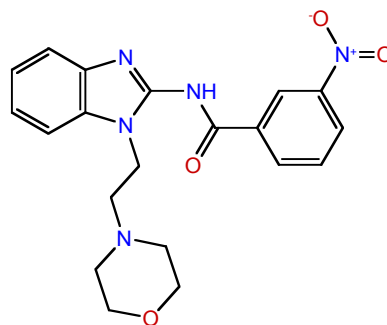
IC261 186611-52-9



CK1

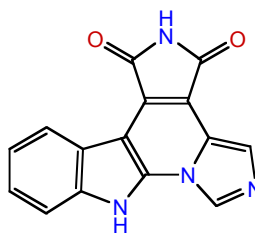
IGF-1R Inhibitor II	196868-63-0		TK
IKK-2 Inhibitor IV	507475-17-4		OTHER
Imatinib	220127-57-1		TK
Indirubin Derivative E804	854171-35-0		CMGC, TK
Indirubin-3'-monoxime	160807-49-8		CMGC

IRAK-1/4 Inhibitor 509093-47-4

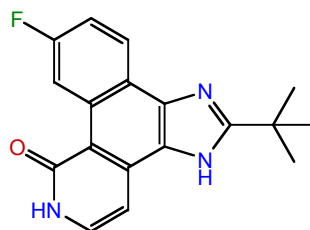


TKL

Isogranulatimide 244148-46-7

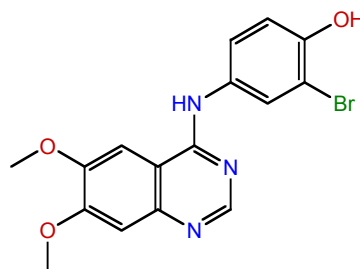
CAMK,
CMGC,
ATYPICAL

JAK Inhibitor I 457081-03-7



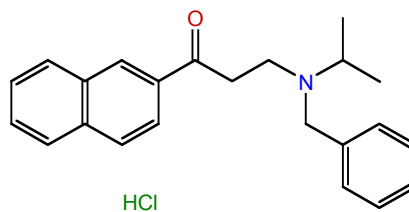
TK

JAK3 Inhibitor II 211555-04-3

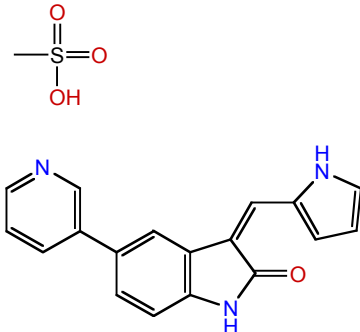
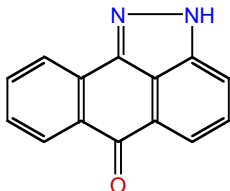
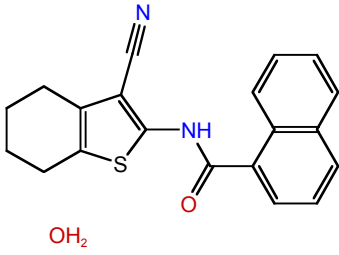
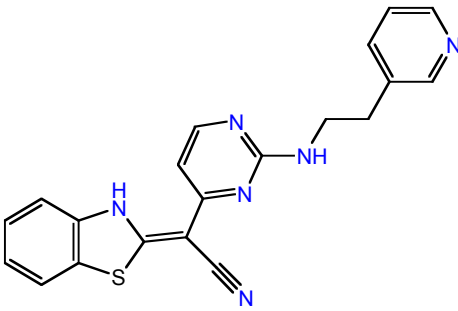
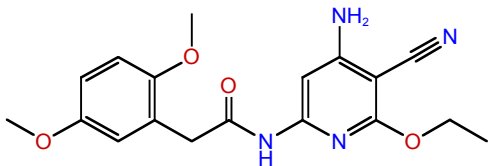


TK

JAK3 Inhibitor IV 58753-54-1

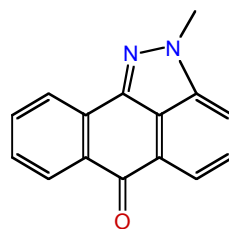


TK

JAK3 Inhibitor VI	856436-16-3	 <chem>COS(=O)(=O)c1ccc2c(c1)c3ccn3c2c4ccn4</chem>	TK
JNK Inhibitor II	129-56-6	 <chem>O=C1c2ccncc2-c3ccccc13</chem>	CMGC
JNK Inhibitor IX	312917-14-9	 <chem>O=C(NC1=CC=C2C=CC=CC12)C3=C(C#N)SC4CCCCC34</chem>	CMGC
JNK Inhibitor V	345987-15-7	 <chem>N#CC1=C(C2=CC=CC=C2S1)C3=CC=NC=C3NCCC4=CC=CC=N4</chem>	CMGC
JNK Inhibitor VIII	894804-07-0	 <chem>CCOC1=CC=C(OC)C(OC)=C1CCC(=O)Nc2cc(C#N)c(N)c2OCC</chem>	CMGC

JNK Inhibitor,
Negative Control

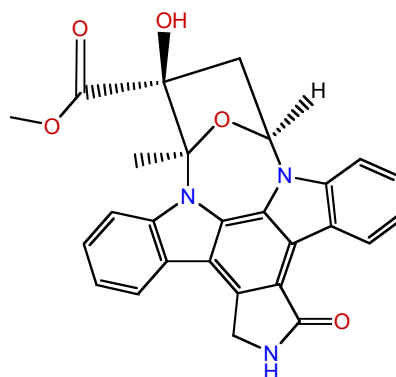
54642-23-8



INACTIVE

K-252a,
Nocardiosis sp.

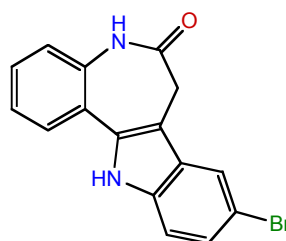
97161-97-2



AGC

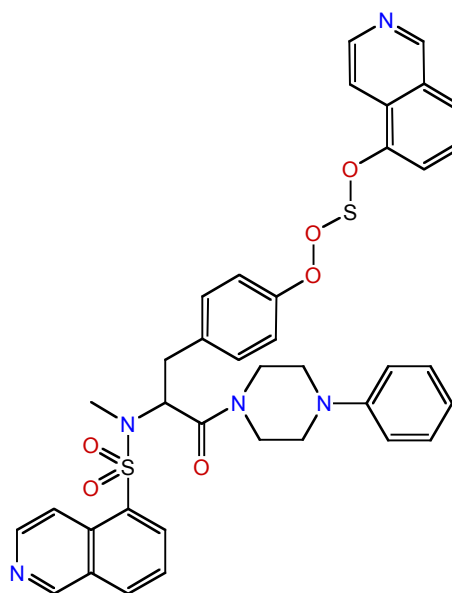
Kenpaullone

142273-20-9

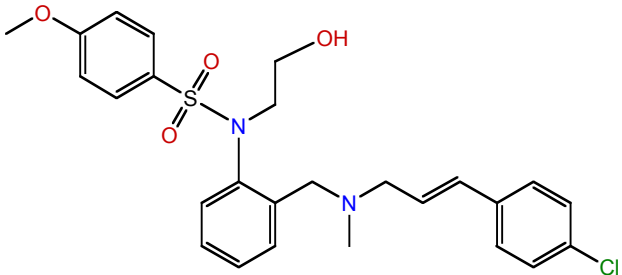
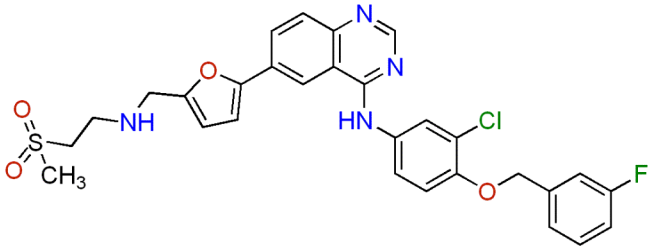
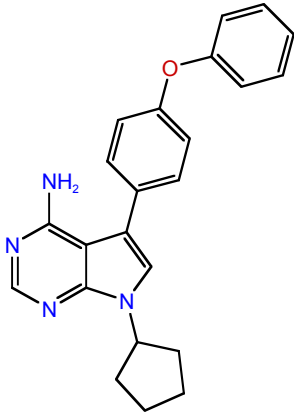
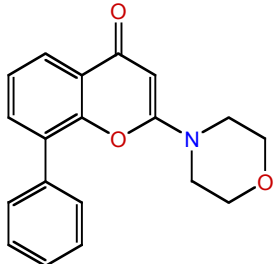
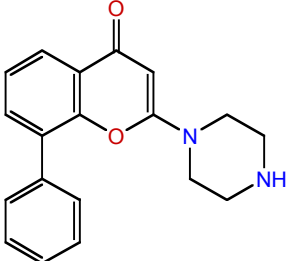
CMGC, CK1,
TK

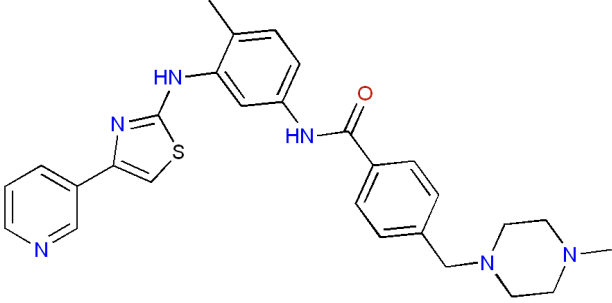
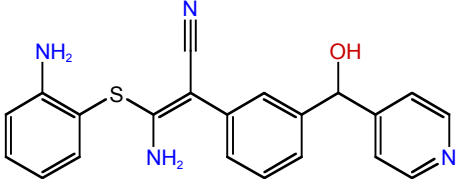
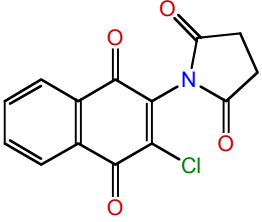
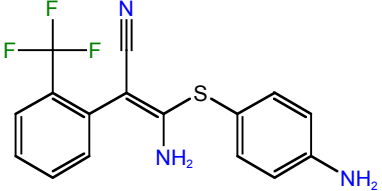
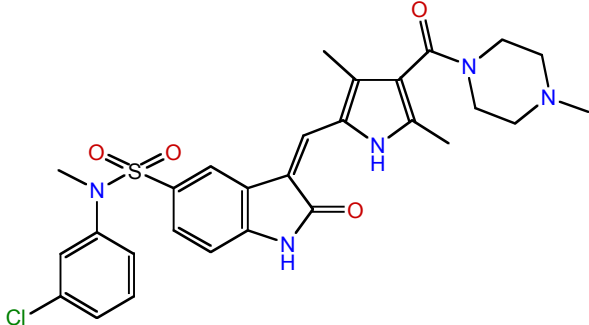
KN-62

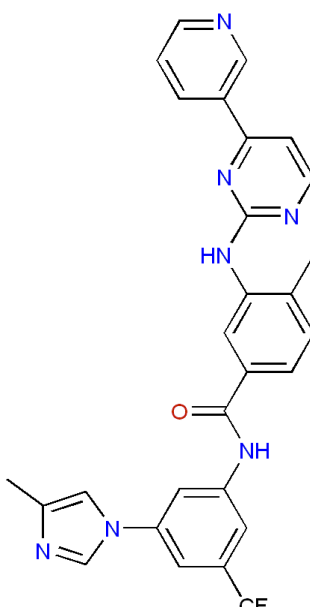
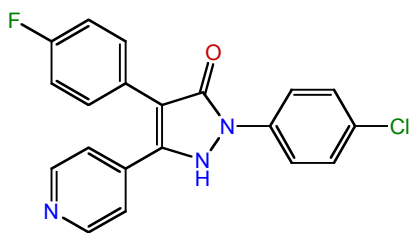
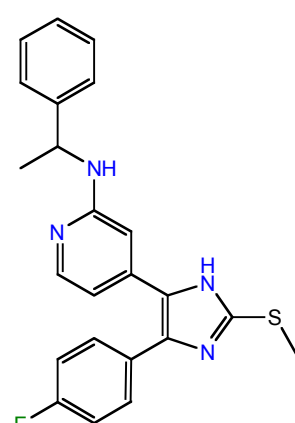
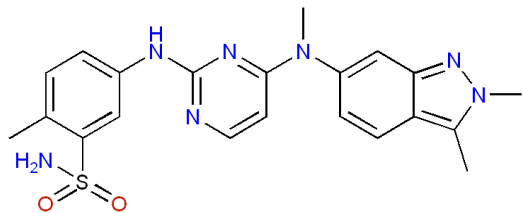
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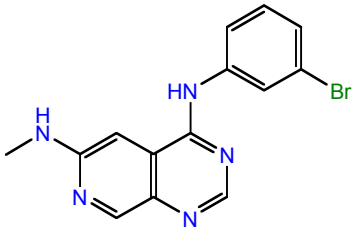
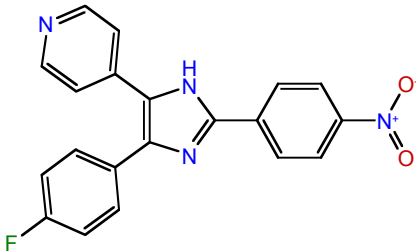
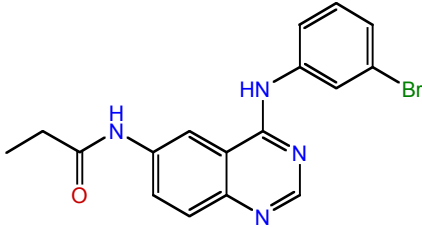
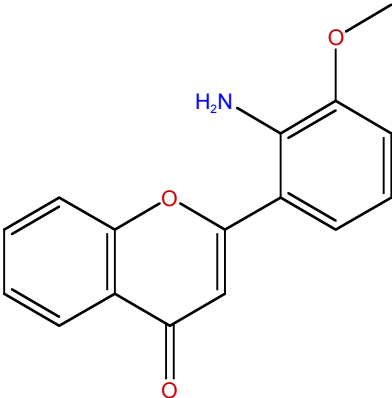
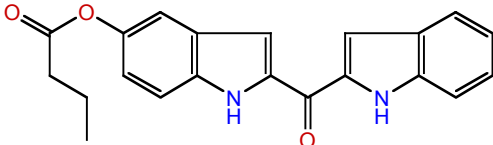


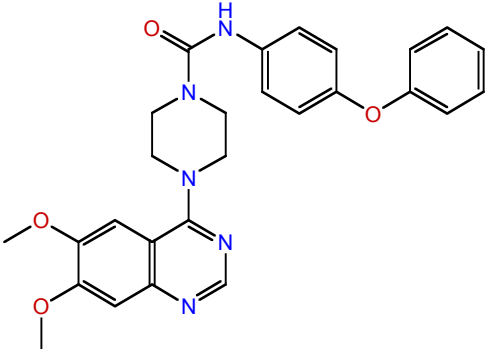
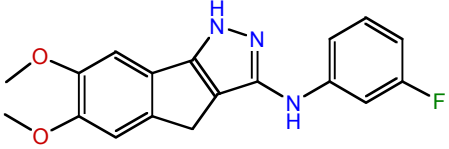
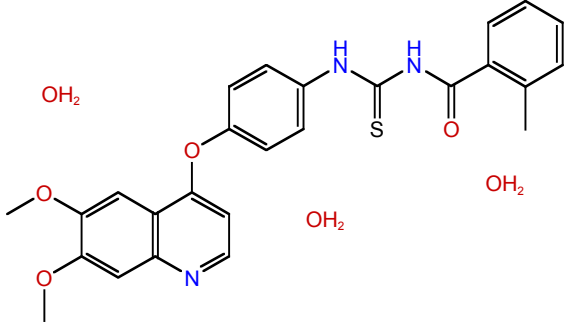
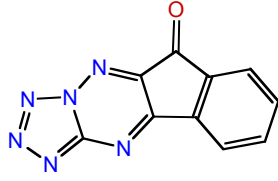
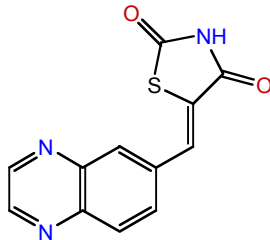
CAMKII

KN-93	139298-40-1	 Chemical structure of KN-93, a protein kinase inhibitor. It features a central benzene ring with a methoxy group at the para position and a propyl chain at the other para position. The propyl chain is substituted with a hydroxyl group at the end and a secondary amine at the middle carbon. This secondary amine is further substituted with a methyl group and a propyl chain that ends in a trans-alkene, which is connected to a 4-chlorophenyl ring.
Lapatinib	231277-92-2	 Chemical structure of Lapatinib, a tyrosine kinase inhibitor. It consists of a central benzimidazole ring system. One of the benzimidazole nitrogens is substituted with a propyl chain ending in a methylsulfonamide group. The other benzimidazole nitrogen is substituted with a propyl chain that is further substituted with a chlorine atom and a methoxy group. The methoxy group is connected to a 4-fluorophenyl ring.
Lck Inhibitor	213743-31-8	 Chemical structure of an Lck inhibitor. It features a central benzimidazole ring system. One of the benzimidazole nitrogens is substituted with a propyl chain ending in a primary amine group. The other benzimidazole nitrogen is substituted with a propyl chain that is further substituted with a cyclopentyl ring and a propyl chain ending in a phenoxy group.
LY 294002	154447-36-6	 Chemical structure of LY 294002, a phosphoinositide 3-kinase inhibitor. It consists of a central benzimidazole ring system. One of the benzimidazole nitrogens is substituted with a propyl chain ending in a carbonyl group. The other benzimidazole nitrogen is substituted with a propyl chain that is further substituted with a benzyl group and a morpholine ring.
LY 303511- Negative control	154447-38-8	 Chemical structure of LY 303511- Negative control, a phosphoinositide 3-kinase inhibitor. It consists of a central benzimidazole ring system. One of the benzimidazole nitrogens is substituted with a propyl chain ending in a carbonyl group. The other benzimidazole nitrogen is substituted with a propyl chain that is further substituted with a benzyl group and a piperidine ring.

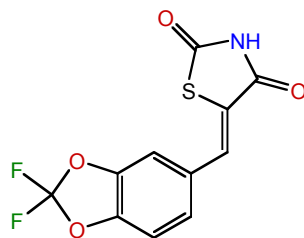
Masitinib	790299-79-5		TK
MEK Inhibitor I	297744-42-4		STE
MEK Inhibitor II	623163-52-0		STE
MEK1/2 Inhibitor	305350-87-2		STE
Met Kinase Inhibitor	658084-23-2		TK

Nilotinib	641571-10-0	 <chem>Cc1ccc(cc1NC(=O)Nc2ccc(C)c2)c3nc4ccc(N)cc4n3</chem>	TK
p38 MAP Kinase Inhibitor	219138-24-6	 <chem>C1=CC=C(C=C1)N2C(=O)C(=C3C=CC(=C3)F)C4=CC=CC=C4N2</chem>	CMGC
p38 MAP Kinase Inhibitor III	581098-48-8	 <chem>CSC1=NC(=C2C=C(C=C2)F)C(=C3C=CC(=C3)N)N1C(=O)C(C)Nc4ccccc4</chem>	CMGC
Pazopanib	444731-52-6	 <chem>Cc1nc2ccc(NC(=O)Nc3ccc(C)cc3)cc2n1</chem>	TK

PD 158780	171179-06-9		TK
PD 169316	152121-53-4		CMGC
PD 174265	216163-53-0		TK
PD 98059	167869-21-8		STE
PDGF Receptor Tyrosine Kinase Inhibitor II	249762-74-1		TK

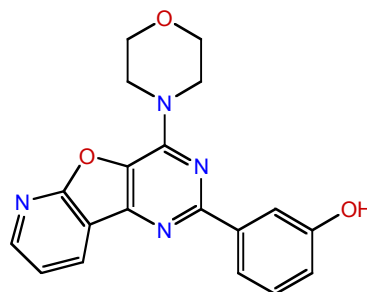
PDGF Receptor Tyrosine Kinase Inhibitor III	205254-94-0	 <chem>COC1=CC=C2C(=C1)N=CN=C2N3CCN(CC3)C(=O)Nc4ccc(Oc5ccccc5)cc4</chem>	TK
PDGF Receptor Tyrosine Kinase Inhibitor IV	627518-40-5	 <chem>COC1=CC=C2C(=C1)C=C(C2)C(=N)Nc3ccc(F)cc3</chem>	TK
PDGF RTK Inhibitor	347155-76-4	 <chem>COC1=CC=C2C(=C1)N=CN=C2Oc3ccc(O)cc3NC(=S)NC(=O)c4cc(O)ccc4</chem>	TK
PDK1/Akt/Fit Dual Pathway Inhibitor	331253-86-2 and 329710-24-9	 <chem>O=C1C=Cc2ccccc2N1N3N=NN3</chem>	AGC, ATYPICAL, TK
PI 3-Kg Inhibitor	648450-29-7	 <chem>O=C1NC(=O)S1C=Cc2ccc3ncnc3c2</chem>	LIPID

PI 3-Kg Inhibitor II 648449-76-7



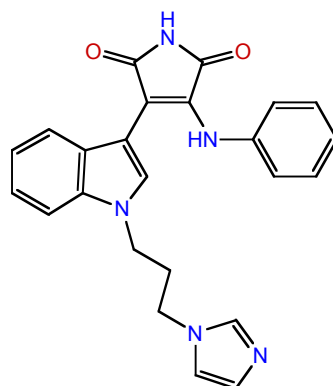
LIPID

PI-103 371935-74-9



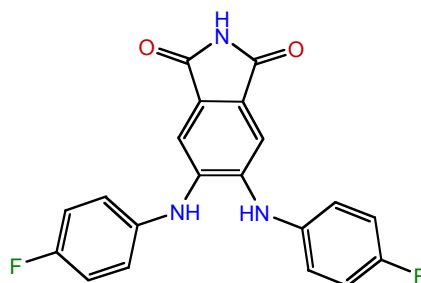
LIPID

PKCb Inhibitor 257879-35-9



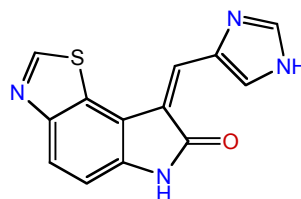
AGC

PKCbII/EGFR Inhibitor 145915-60-2



TK, AGC

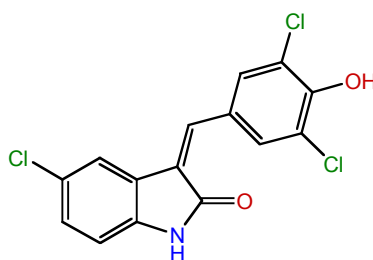
PKR Inhibitor 608512-97-6



OTHER

PKR Inhibitor,
Negative Control

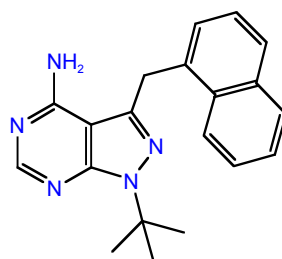
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INACTIVE

PP1 Analog II,
1NM-PP1

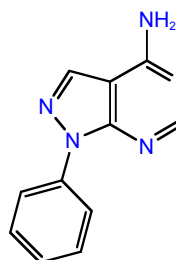
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TK

PP3

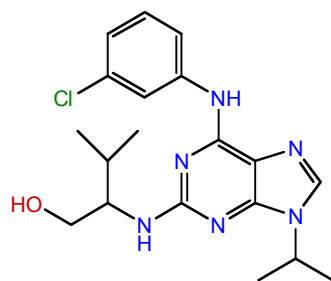
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TK

Purvalanol A

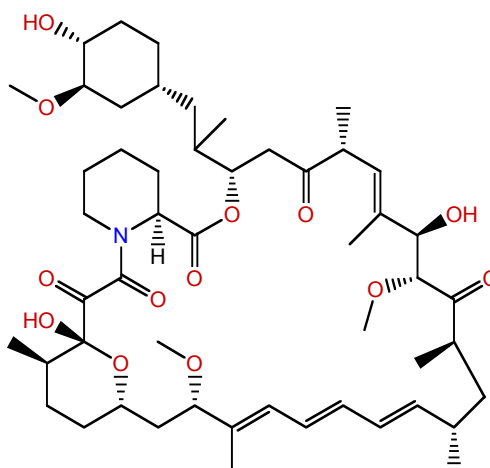
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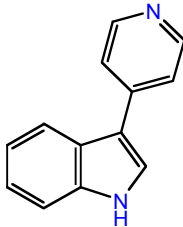
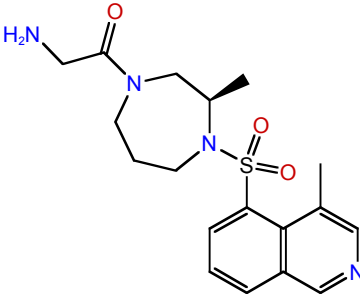
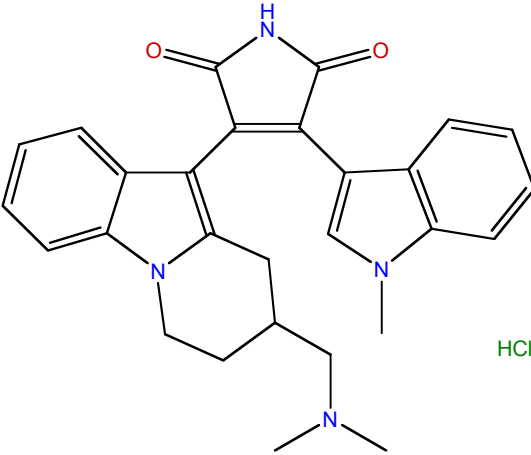
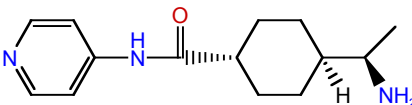
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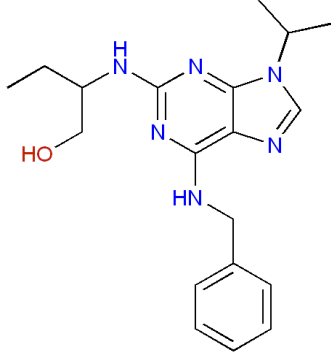
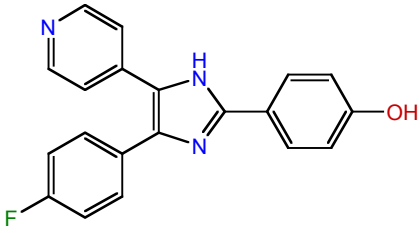
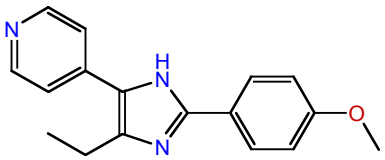
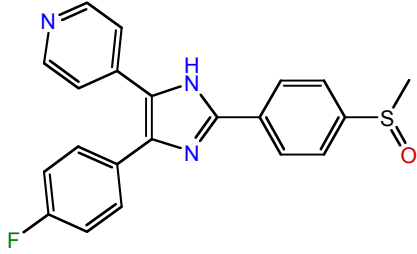
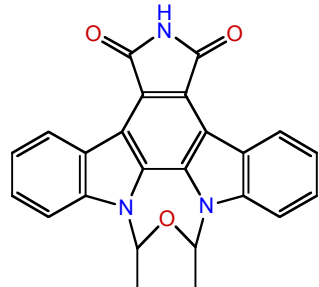
Rapamycin

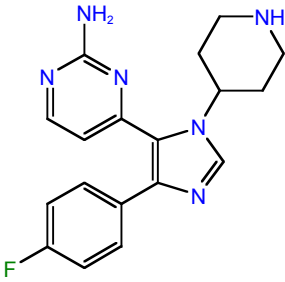
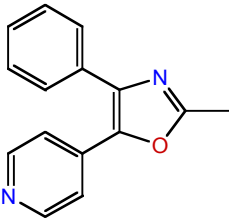
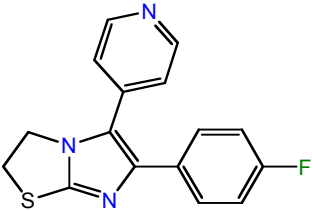
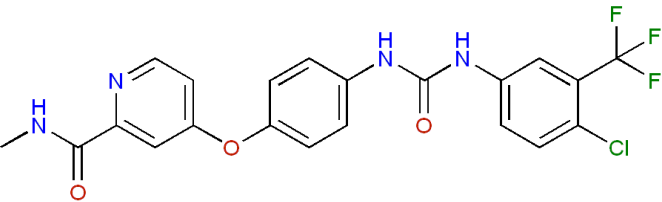
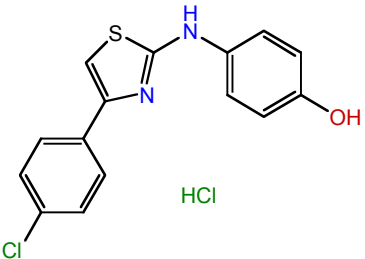
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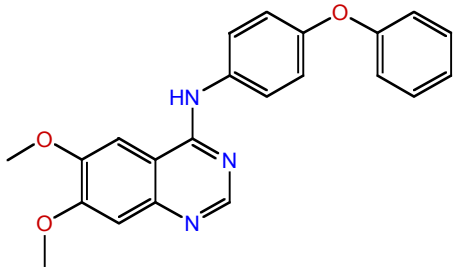
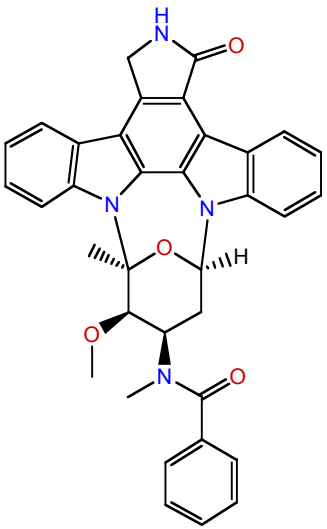
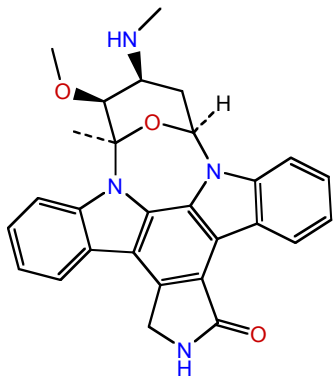
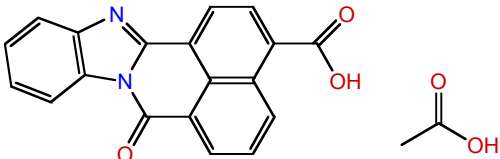


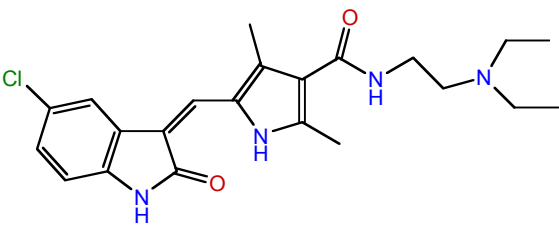
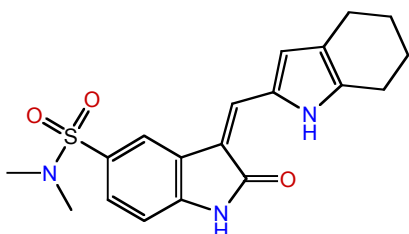
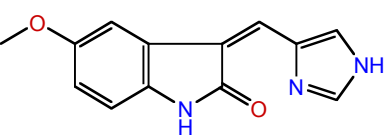
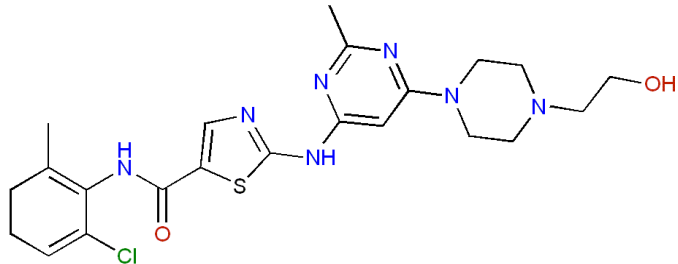
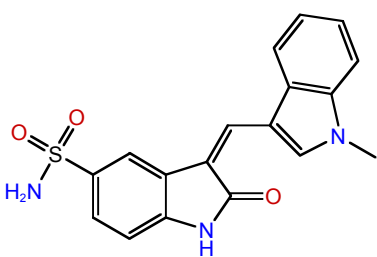
AGC

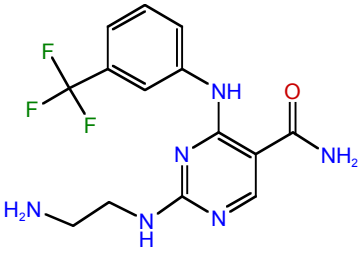
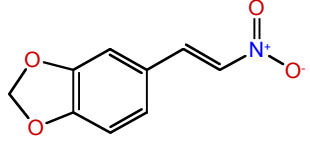
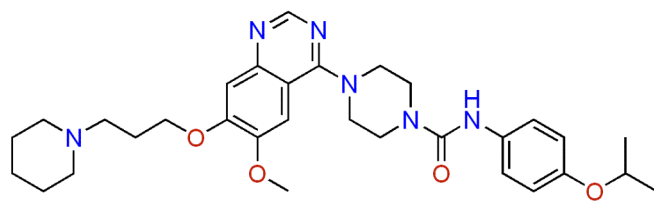
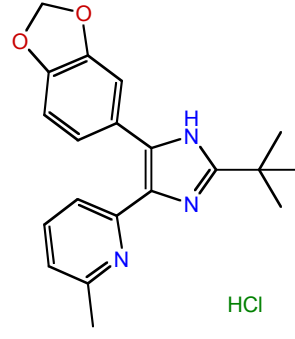
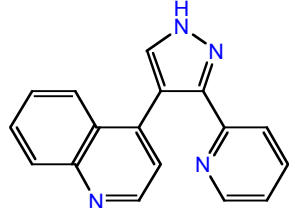
Rho Kinase Inhibitor III, Rockout	7272-84-6		AGC
Rho Kinase Inhibitor IV	913844-45-8		AGC
Ro-32-0432	151342-35-7	 HCl	AGC
ROCK Inhibitor, Y-27632	146986-50-7	 HCl HCl OH ₂	AGC

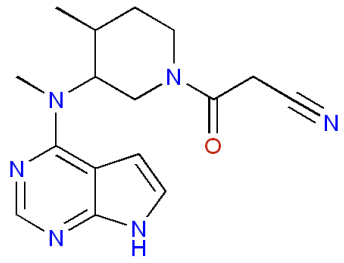
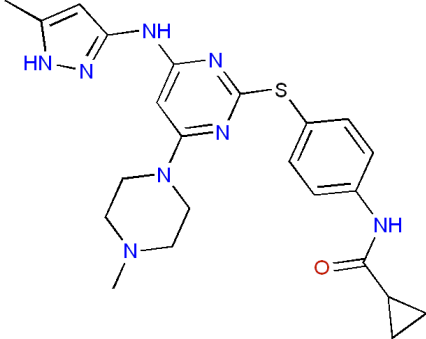
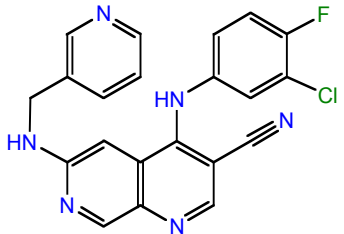
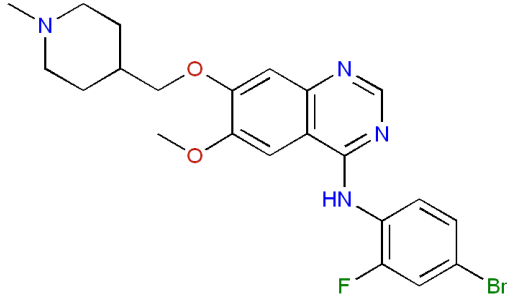
Roscovitine	186692-46-6		CMGC
SB 202190	152121-30-7		CMGC
SB 202474, Negative control for p38 MAPK inhibition studies	172747-50-1		INACTIVE
SB 203580	152121-47-6		CMGC
SB 218078	135897-06-2		CAMK

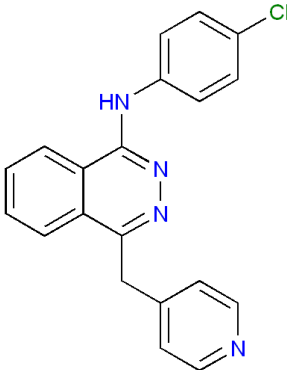
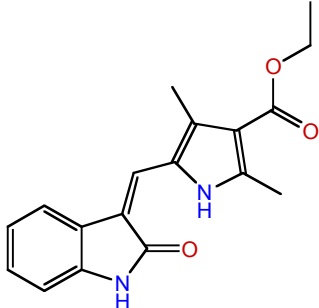
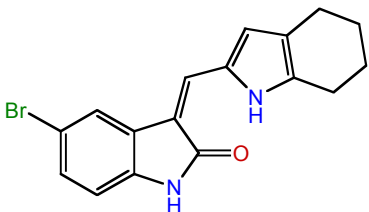
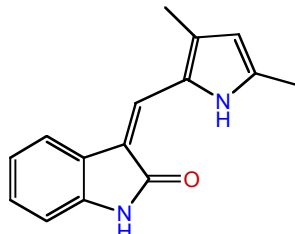
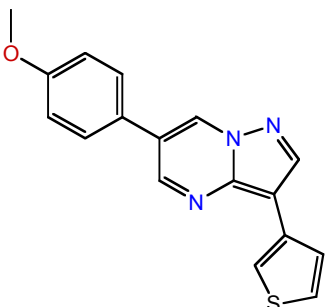
SB220025	165806-53-1		CMGC
SC-68376	318480-82-9		CMGC
SKF-86002	72873-74-6		CMGC
Sorafenib	284461-73-0		TK
Sphingosine Kinase Inhibitor	312636-16-1		LIPID

Src Kinase Inhibitor I	179248-59-0		TK
Staurosporine, N-benzoyl-	120685-11-2		AGC, CMGC, TK
Staurosporine, Streptomyces sp.	62996-74-1		AGC, CAMK, TK
STO-609	52029-86-4		CAMK

SU11652	326914-10-7		TK
SU6656	330161-87-0		TK
SU9516	666837-93-0		CMGC
Sunitinib	557795-19-4		TK
Syk Inhibitor	622387-85-3		TK

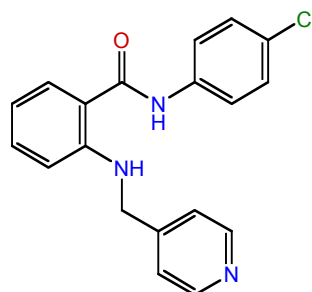
Syk Inhibitor II	227449-73-2		OH_2 OH_2 HCl HCl	TK
Syk Inhibitor III	1485-00-3			TK
Tandutinib	387867-13-2			TK
TGF-b RI Inhibitor III	356559-13-2		HCl	TKL
TGF-b RI Kinase Inhibitor	396129-53-6			TKL

Tofacitinib	477600-75-2	 <chem>CN1CCN(C1)C2=CN3C=CC=C3N2C(=O)CC#N</chem>	TK
Tozasertib	639089-54-6	 <chem>CN1CCN(C1)C2=CN3C=CC=C3N2S4=CC=C(C=C4)NC(=O)C5CC5</chem>	OTHER
Tpl2 Kinase Inhibitor	871307-18-5	 <chem>C#Nc1nc2nc3c(nc12)ncn3C4=CC=C(C=C4)N5C=CC=C5F</chem>	CMGC
Vandetanib	443913-73-3	 <chem>COC1=CC=C(C=C1OC2=CC=NC=C2NC3=CC=C(C=C3)F)C4=CC=CC=C4Br</chem>	TK

Vatalanib	212141-51-0		TK
VEGF Receptor 2 Kinase Inhibitor I	15966-93-5		TK
VEGF Receptor 2 Kinase Inhibitor II	288144-20-7		TK
VEGF Receptor 2 Kinase Inhibitor III	204005-46-9		TK
VEGF Receptor 2 Kinase Inhibitor IV	216661-57-3		TK

VEGF Receptor
Tyrosine Kinase
Inhibitor II

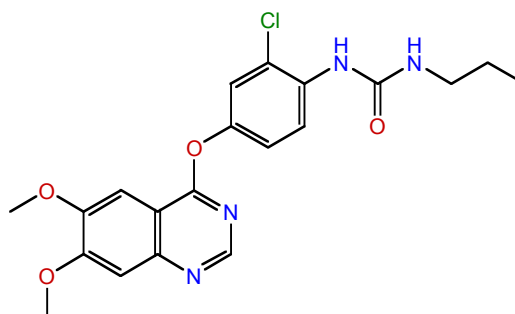
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TK

VEGF Receptor
Tyrosine Kinase
Inhibitor III, KRN633

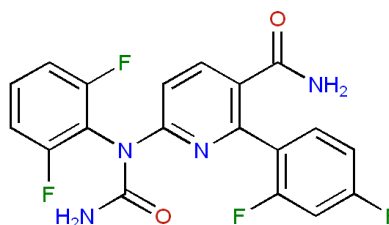
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TK

VX-702

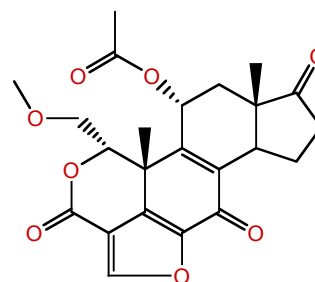
745833-23-2



CMGC

Wortmannin

19545-26-7



ATYPICAL

Supplementary Table 2. Kinase constructs and substrates used in this study.

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
ABL1	ABL1	Abltide	NP_005148.2	P00519	full-length	-	baculovirus in Sf21 insect cells	C-terminal His
ABL2/ARG	ABL2	Abltide	NP_009298	P42684	full-length	-	baculovirus in Sf21 insect cells	C-terminal His
ACK1	TNK2	Abltide	NP_005772.3	Q07912	aa 110-476	-	baculovirus in Sf21 insect cells	N-terminal GST
AKT1	AKT1	Crosstide	NP_005154	P31749	full-length		baculovirus in Sf21 insect cells	N-terminal His
AKT2	AKT2	Crosstide	NP_001617	P31751	full-length		baculovirus in Sf21 insect cells, activated by PDK1	N-terminal His
AKT3	AKT3	Crosstide	NP_005456	Q9Y243	full-length		baculovirus in Sf21 insect cells	N-terminal His
ALK	ALK	pEY	NP_004295.2	Q9UM73	cytoplasmic	-	Insect	N-terminal GST
ALK1/ACVRL1	ACVRL1	Casein	NP_000011.2	P37023	cytoplasmic aa139-503	-	Insect	N-terminal GST
ALK2/ACVR1	ACVR1	Casein	NP_001096.1	Q04771	cytoplasmic aa145-509	-	Insect	N-terminal GST
ALK4/ACVR1B	ACVR1B	Casein	NP_004293	P36896	aa 150-505	-	Baculovirus infected insect cells	N-terminal GST
ALK5/TGFBR1	TGFBR1	Casein	NM_004612	P36897	aa200-503	-	Sf9 cells	GST-HIS fusion
ARAF	ARAF	MEK1 (K97R)	NM_001654	P10398	aa 282-end	YY301-302DD	Baculovirus infected Sf9 cells	N-terminal GST-tag
ARK5/NUAK1	NUAK1	CHKtide	NP_055655	O60285	full-length	-	Insect	N-terminal His
ASK1/MAP3K5	MAP3K5	MBP	NP_005914	O99683	full-length	-	Insect	N-terminal GST
Aurora A	AURKA	Kemptide	NP_940839	O14965	full length	-	baculovirus in Sf21 insect cells	N-terminal His6-tag
Aurora B	AURKB	Kemptide	NP_004208.2	Q96GD4	full-length	-	Insect	N-terminal His
Aurora C	AURKC	Kemptide	AAH75064, NP_003151	Q9UQB9	full-length	-	Insect	N-terminal His

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
AXL	AXL	Abltide + Mn	NP_068713	P30530	aa 473-894	-	Baculovirus infected Sf9 cells	C-terminal His
BLK	BLK	pEY	NP_001706	P51451	full-length	-	Insect	N-terminal His
BMX/ETK	BMX	pEY	NP_001712	P51813	full length	-	baculovirus in Sf21 insect cells	C-terminal His
BRAF	BRAF	MEK1 (K97R)	NP_004324.2	P15056	full-length	-	Insect	N-terminal GST
BRK	PTK6	pEY + Mn	NP_005966	Q13882	full-length	-	Insect	C-terminal His
BRSK1	BRSK1	CHKtide	NP_115806	Q8TDC3	full-length	-	Insect	N-terminal GST-tag
BRSK2	BRSK2	ZIptide	GenBank NM_003957	Q8IWQ3	full-length	-	baculovirus in Sf21 insect cells	N-terminal His6-tag
BTK	BTK	pEY	NP_000052	Q06187	full-length	-	Insect	N-terminal His6-tagged
CAMK1a	CAMK1	Autocamtide 2 + Ca-CaM	NP_003647.1	Q14012	full length	-	baculovirus insect cell	N-terminal His-tag
CAMK1b	PNCK	Autocamtide 2 + Ca-CaM	GenBank NM_012040	Q6P2M8	full length	-	baculovirus insect cell	N-terminal GST-tag
CAMK1d	CAMK1D	Autocamtide 2 + Ca-CaM	NP_705718.1	Q8IU85	full length	-	baculovirus insect cell	N-terminal His-tag
CAMK1g	CAMK1G	Autocamtide 2 + Ca-CaM	GenBank NM_020439	Q96NX5	C-terminal truncation	-	baculovirus insect cell	N-terminal GST-tag
CAMK2a	CAMK2A	Autocamtide 2 + Ca-CaM	NP_741960	Q9UQM7	full length	-	baculovirus insect cell	C-terminal His-tag
CAMK2b	CAMK2B	Autocamtide 2 + Ca-CaM	NP_742078.1	Q13554	full length	-	baculovirus insect cell	N-terminal His6-tag
CAMK2d	CAMK2D	ZIptide + Ca-CaM*	NP_742113	Q13557	full length	-	baculovirus insect cell	C-terminal His6-tag
CAMK2g	CAMK2G	ZIptide + Ca-CaM*	GenBank NM_172169	Q13555	C-terminal truncation	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
CAMK4	CAMK4	ZIptide + Ca-CaM*	NP_001735	Q9UQM7	full length	-	E. coli	N-terminal GST-tag
CAMKK1	CAMKK1	MBP + Ca-CaM	GenBank NM_032294	Q8N5S9	full-length	-	baculovirus in Sf9 insect cells	N-terminal GST

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CAMKK2	CAMKK2	MBP + Ca-CaM	NP_757380.1	Q96RR4	full-length	-	Baculovirus infected insect cells	N-terminal GST
CDK1/cyclin A	CDK1/CCNA2	Histone H1	NM_001786/ NM_001237	CDK1: P06493; cyclin A: P20248	full length / full length	-	baculovirus in Sf9 insect cells	N-terminal GST-tag / N-terminal GST-tag
CDK1/cyclin B	CDK1/CCNB1	Histone H1	NP_001777/B P_114172	CDK1: P06493; cyclin B: P14635	full length / full length	-	baculovirus insect cell	C-terminal His6-tag / N-terminal His6-tag
CDK2/cyclin A	CDK2/CCNA2	Histone H1	NP_001789, NP_001228	CDK2: P24941; cyclin A: P20248	full-length	-	Insect	N-terminal His6-tag / N-terminal His6-tag
CDK2/cyclin E	CDK2/CCNE1	Histone H1	EMBL M68520, GenBank NM_001238	CDK2: P24941; cyclin E: P24864	full length / full length	-	baculovirus in Sf21 insect cells	C-terminal His6-tag / N-terminal GST-tag
CDK3/cyclin E	CDK3/CCNE1	Histone H1	NM_001258, NM_001238	CDK3: Q00526; cyclin E: P24864	full length / full length	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
CDK4/cyclin D1	CDK4/CCND1	RB-CTF	NP_000066, NP_444284	CDK4: P11802; Cyclin D1: P24385	full length	-	baculovirus insect cell	N-terminal GST-tag
CDK4/cyclin D3	CDK4/CCND3	RB-CTF	NM_000075, NM_001760	CDK4: P11802; Cyclin D3: P30281	full length	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
CDK5/p25	CDK5/CDK5R1	Histone H1	NP_004926.1, NP_003876	CDK5: Q00535; p25: Q15078	full length / full length	-	baculovirus insect cell	N-terminal His6-tag / N-terminal GST-tag

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CDK5/p35	CDK5/CDK5R1	Histone H1	NP_004926.1, NP_003876	CDK5: Q00535; p35: Q15078	full length / full length	-	baculovirus insect cell	N-terminal His6-tag / N-terminal His6-tag
CDK6/cyclin D1	CDK6/CCND1	RB-CTF	NP_001250, NP_444284	CDK6: Q00534; Cyclin D1: P24385	full-length	-	Baculovirus infected insect cells	N-terminal GST
CDK6/cyclin D3	CDK6/CCND3	RB-CTF	X66365, M90814	CDK6: Q00534; Cyclin D3: P30281	full length / full length	-	baculovirus in Sf9 insect cells	N-terminal His6-tag / N-terminal GST-tag
CDK7/cyclin H	CDK7/CCNH/MNAT1	Histone H1	NP_001790, NP_001230, NP_002422.1	CDK7: P50613; Cyclin H: P51946; MNAT1: Q6ICQ7	full-length	-	Insect	N-terminal His
CDK9/cyclin K	CDK9/CCNK	PDKtide	NP_001252, NP_003849	CDK9: P50750; Cyclin K: O75909	full length / full length	-	Insect	N-terminal His6-tag / N-terminal His6-tag
CDK9/cyclin T1	CDK9/CCNT1	PDKtide	NP_001252, NP_001231	CDK9: P50750; Cyclin T1: O60563	full-length	-	Insect	N-terminal His
CHK1	CHEK1	CHKtide	GenBank NM_001274	O14757	full length	-	baculovirus in Sf9 insect cells	N-terminal His
CHK2	CHEK2	CHKtide	NP_009125	O96017	full-length	-	baculovirus in Sf21 insect cells	C-terminal His
CK1a1	CSNK1A1	CK1tide	NP_001883.4	P48729	full length	-	baculovirus insect cell	GST-tag
CK1d	CSNK1D	CK1tide	NP_620693	P48730	full length	-	baculovirus insect cell	N-terminal GST-tag
CK1epsilon	CSNK1E	CK1tide	NP_001885	P49674	full length	-	baculovirus insect cell	C-terminal His-tag
CK1g1	CSNK1G1	CK1tide	NP_071331	Q9HCP0	full-length	-	Insect	N-terminal GST

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CK1g2	CSNK1G2	CK1tide	NP_001310	P78368	full length	-	baculovirus insect cell	C-terminal His-tag
CK1g3	CSNK1G3	CK1tide	NP_004375.1, NP_004375.2	Q9Y6M4	full-length	-	Insect	N-terminal GST
CK2a	CSNK2A1	CK2 sub	NP_001886	P68400	full length	-	baculovirus insect cell	C-terminal GST-tag
CK2a2	CSNK2A2	CK2 sub	NP_001887	P19784	full length	-	baculovirus insect cell	N-terminal GST-tag
c-Kit	KIT	pEY + Mn	NP_000213	P10721	aa 544-976	-	Insect	His6-tag
CLK1	CLK1	MBP	NP_004062	P49759	full catalytic domain	-	E. coli	N-terminal GST
CLK2	CLK2	MBP	NP_003984	P49760	catalytic domain aa137-498	-	baculovirus insect cell	N-terminal GST
CLK3	CLK3	MBP	NP_003983	P49761	full-length	-	Insect	N-terminal GST
CLK4	CLK4	MBP	NP_065717	Q9HAZ1	full-length	-	Insect	N-terminal GST
c-MER	MERTK	pEY	NP_006334.2	Q12866	aa 578-872	-	baculovirus insect cell	N-terminal GST
c-MET	MET	MBP	NP_000236.2	P10721	aa 956-1390	-	baculovirus insect cell	N-terminal His
COT1/MAP3K ₈	MAP3K8	MEK1 (K97R)	NP_005195	P41279	aa 30-397	-	Baculovirus infected insect cells	N-terminal GST
CSK	CSK	pEY	NP_004374	P41240	full-length	-	E. coli	C-terminal His
c-Src	SRC	pEY	NP_005408	P12931	full-length	-	Insect	C-terminal His
CTK/MATK	MATK	pEY	NP_647611	P42679	full-length	-	Insect	C-terminal His
DAPK1	DAPK1	ZIPtide	NP_004929	P53355	full catalytic	-	Insect	N-terminal GST
DAPK2	DAPK2	ZIPtide + Ca-CaM	NP_055141	Q9UIK4	full catalytic	-	Insect	N-terminal GST
DCAMKL2	DCLK2	Autocamtide 2 + Ca-CaM	NP_689832	Q8N568	full-length	-	Baculovirus infected insect cells	N-terminal GST
DDR2	DDR2	AXLtide + Mn	NP_006173.2	Q16832	aa 424-855	-	baculovirus in insect cells	N-terminal GST

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DMPK	DMPK	AXLtide	NP_004400	Q09013	full-length	-	Insect	N-terminal GST
DRAK1/STK17A	STK17A	ZIPtide	NP_004751	Q9UEE5	full-length	-	Insect	N-terminal GST
DYRK1/DYRK1A	DYRK1A	Casein	NP_001387	Q13627	full-length	-	Insect	N-terminal GST
DYRK1B	DYRK1B	Casein	NP_004705	Q9Y463	full-length	-	Insect	N-terminal GST
DYRK2	DYRK2	Casein	GenBank NM_003583	Q92630	full length	-	baculovirus in Sf21 insect cells	His6-tag
DYRK3	DYRK3	Casein	NP_003573	O43781	full length	-	Insect	N-terminal GST
DYRK4	DYRK4	Casein	NP_003836.1	Q9NR20	full length	-	Insect	N-terminal GST
EGFR	EGFR	pEY + Mn	NP_005219.2	P00533	cytoplasmic	-	Insect	N-terminal GST
EPHA1	EPHA1	pEY + Mn	NP_005223.2	P21709	cytoplasmic	-	Insect	N-terminal GST
EPHA2	EPHA2	pEY	NP_004422.2	P29317	cytoplasmic	-	Insect	N-terminal GST
EPHA3	EPHA3	pEY + Mn	NP_005224	P29320	cytoplasmic	-	Insect	C-terminal His
EPHA4	EPHA4	pEY + Mn	NP_004429.1	P54764	aa 616-887	-	baculovirus in insect cells	N-terminal GST
EPHA5	EPHA5	pEY + Mn	NP_004430.1	P54756	aa 595-1037	-	baculovirus in insect cells	N-terminal GST
EPHA6	EPHA6	pEY	NM_001080448	Q9UF33	Catalytic (561-end)	-	Insect	N-terminal GST
EPHA7	EPHA7	pEY	NP_004431.1	Q15375	catalytic domain (aa 579-998)	-	baculovirus insect cell	N-terminal GST-tag
EPHA8	EPHA8	pEY	NP_065387	P29322	catalytic domain (aa 565-1005)	-	baculovirus insect cell	N-terminal GST-tag
EPHB1	EPHB1	pEY	NP_004432	P54762	cytoplasmic	-	Insect	N-terminal GST
EPHB2	EPHB2	pEY + Mn	NP_004433	P29323	aa 616-889	-	Insect	GST
EPHB3	EPHB3	pEY	NP_004434	P54753	cytoplasmic	-	Insect	N-terminal GST
EPHB4	EPHB4	pEY	NP_004435	P54760	cytoplasmic	-	Insect	C-terminal His
ERBB2/HER2	ERBB2	pEY + Mn	GenBank X03363	P04626	aa679-1255	-	Insect	N-terminal GST
ERBB4/HER4	ERBB4	pEY + Mn	NP_005226	Q15303	aa 708-993	-	baculovirus insect cell	N-terminal GST
ERK1/MAPK3	MAPK3	MBP	NP_002737	P27361	full-length	-	Insect	N-terminal GST

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ERK2/MAPK1	MAPK1	MBP	NP_620407	P28482	full-length	-	E. coli	N-terminal GST
FAK/PTK2	PTK2	pEY	NP_722560	Q05397	full-length	-	Insect	N-terminal GST
FER	FER	pEY	NP_005237	P16591	aa540-822	-	baculovirus insect cell	N-terminal GST
FES/FPS	FES	pEY	NP_001996	P07332	full-length	-	Insect	C-terminal His
FGFR1	FGFR1	pEY + Mn	NP_000595	P11362	cytoplasmic	-	Insect	C-terminal His
FGFR2	FGFR2	pEY + Mn	NP_075261	P21802	cytoplasmic	-	Insect	C-terminal His
FGFR3	FGFR3	pEY + Mn	NP_000133	P22607	cytoplasmic	-	Insect	N-terminal His
FGFR4	FGFR4	pEY + Mn	NP_002002	P22455	aa 460-802	-	baculovirus insect cell	N-terminal His6-tag
FGR	FGR	pEY	NP_005239	P09769	full-length	-	baculovirus insect cell	C-terminal His6-tag
FLT1/VEGFR 1	FLT1	pEY + Mn	NP_002010	P17948	aa 781-1338	-	baculovirus insect cell	N-terminal GST tagged
FLT3	FLT3	Abltide	NP_004110	P36888	aa 564-958	-	baculovirus insect cell	C-terminal His6-tag
FLT4/VEGFR 3	FLT4	pEY + Mn	NP_891555.1, AAA85215	P35916	aa 800-1297	Q890H	Insect	N-terminal GST
FMS	CSF1R	pEY + Mn	NP_005202	P07333	cytoplasmic	-	Insect	C-terminal His
FRK/PTK5	FRK	pEY + Mn	NP_002022	P42685	full-length	-	Insect	N-terminal GST
FYN	FYN	pEY	NP_694592	P06241	full-length	-	Insect	C-terminal His
GCK/MAP4K2	MAP4K2	MBP	NP_004570.2	Q12851	full-length	-	Insect	N-terminal His6-tagged
GRK2	ADRBK1	Casein	AAH37963	P25098	full length	-	baculovirus insect cell	C-terminal His-tag
GRK3	ADRBK2	Casein	NP_005151	P35626	full-length	-	Insect	N-terminal GST
GRK4	GRK4	Casein	NP_892027	P32298	full-length	-	Insect	N-terminal GST
GRK5	GRK5	Casein	NP_005299	P34947	full-length	-	Insect	N-terminal GST
GRK6	GRK6	Casein	NP_001004106	P43250	full-length	-	Insect	N-terminal GST
GRK7	GRK7	Casein	NP_631948	Q8WTQ7	full-length	-	Insect	N-terminal GST
GSK3a	GSK3A	Phospho-Glycogen Synthase peptide	NP_063937.2	P49840	full length	-	baculovirus insect cell	C-terminal His-tag

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GSK3b	GSK3B	Phospho-Glycogen Synthase peptide	NP_002084	P49841	full-length		baculovirus insect cell	C-terminal His6-tag
Haspin	GSG2	Histone H3	NP_114171.1	Q8TF76	aa471-798	-	Insect	C-terminal His
HCK	HCK	Src Substrate peptide	NP_002101	P08631	full-length	-	Insect	C-terminal His
HGK/MAP4K4	MAP4K4	MBP	NP_004825	O95819	full catalytic	-	Insect	N-terminal GST
HIPK1	HIPK1	MBP	NP_689909	Q86Z02	aa 158-555	-	baculovirus insect cell	N-terminal GST
HIPK2	HIPK2	MBP	NP_073577.3	Q9H2X6	aa 165-564	-	baculovirus insect cell	N-terminal GST
HIPK3	HIPK3	MBP	NP_005725.2	Q9H422	aa 163-562	-	baculovirus insect cell	N-terminal His6-tag
HIPK4	HIPK4	MBP	NP_653286	Q8NE63	full-length	-	baculovirus insect cell	N-terminal GST
IGF1R	IGF1R	pEY + Mn	NP_000866	P08069	aa 960-1367	-	baculovirus insect cell	C-terminal His
IKKa/CHUK	CHUK	IKKtide	NP_001269	O15111	full-length	-	Baculovirus infected insect cells	N-terminal 6X-His tag
IKKb/IKBKB	IKBKB	IKKtide	NP_001547	O14920	full-length	-	Insect	N-terminal GST
IKKe/IKBKE	IKBKE	Casein	NP_054721.1	Q14164	full-length	-	Insect	N-terminal GST
IR	INSR	pEY + Mn		P06213	cytoplasmic domain of the β -subunit (aa 941-1343)	-	baculovirus expression system	GST-tag
IRAK1	IRAK1	MBP	NP_001560	P51617	aa 197-721	-	Baculovirus infected insect cells	N-terminal GST
IRAK4	IRAK4	MBP	NP_057207, AAH13316	Q9NWZ3	full-length	-	baculovirus insect cell	N-terminal His6-tag
IRR/INSRR	INSRR	AXLtide	NP_055030	P14616	cytoplasmic	-	Insect	N-terminal GST

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ITK	ITK	MBP	NP_005537	Q08881	full-length	-	Insect	N-terminal GST
JAK1	JAK1	pEY	NP_002218.2	P23458	aa 866-1154	-	Insect	N-terminal GST
JAK2	JAK2	pEY	NP_004963	O60674	aa 809-1132 +g	-	Insect	N-terminal GST
JAK3	JAK3	JAK3tide	NP_000206	P52333	aa 781-1124	-	Insect	N-terminal GST
JNK1	MAPK8	ATF2	NP_002741.1	P45983-2	full length	-	baculovirus insect cell, activated by MAP2K7	N-terminal His-tag
JNK2	MAPK9	ATF2	NP_002743	P45984-1	full length	-	baculovirus in insect cell, activated by MAP2K7	N-terminal His-tag
JNK3	MAPK10	ATF2	NP_002744	P53779	full length	-	baculovirus in insect cell	N-terminal GST
KDR/VEGFR2	KDR	pEY + Mn	NP_002244	P35968	aa 789-1356	-	baculovirus in insect cell, activated by autophosphorylation	C-terminal His6-tagged
KHS/MAP4K5	MAP4K5	MBP	NP_942089	Q9Y4K4	full length	-	baculovirus in insect cell	N-terminal GST
LCK	LCK	pEY + Mn	NP_005347	P06239	full-length	-	baculovirus in insect cells	C-terminal His6-tagged
LIMK1	LIMK1	Cofilin 1	NP_002305	P53667	catalytic domain (aa 285-638)	-	baculovirus in insect cells, activated by co-expression with ROCK1	N-terminal His6-tag
LKB1	STK11/STRADA/CAB39	LKB1tide	NM000455/A F308302/NM_016289	STK11:Q1583 1; STRADA:Q7 RTN6; CAB39:Q9Y3 76	full length	-	baculovirus in Sf21 cells	

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LOK/STK10	STK10	Axltide	GenBank NM_005990	O94804	aa 1-348	-	baculovirus in Sf21 insect cells	N-terminal His6- tag
LRRK2	LRRK2	LRRKtide	NP_940980.2	Q5S007	aa 970-2527	-	baculovirus in insect cells	N-terminal GST
LYN	LYN	pEY	NP_002341	P07948-1	full length	-	baculovirus in insect cells	C-terminal His6- tag
LYN B	LYN	pEY+ Mn	NP_002341	P07948-2	full-length	-	Insect	C-terminal His
MAPKAPK2	MAPKAPK2	Glycogen Synthase- derived peptide	NP_116584	P49137	ful length		E. coli, activated by MAPK14	N-terminal His-tag
MAPKAPK3	MAPKAPK3	Glycogen Synthase- derived peptide	NP_004626	Q16644	full length	-	Insect cell, activated by MAPK14	N-terminal His-tag
MAPKAPK5/P RAK	MAPKAPK5	Glycogen Synthase- derived peptide	NP_003659	Q8IW41	full length	-	baculovirus in insect cells	N-terminal His6- tag
MARK1	MARK1	CHKtide	NP_061120.1	Q9P0L2	full length	-	baculovirus in insect cells	N-terminal GST- tag
MARK2/PAR- 1Ba	MARK2	CHKtide	NP_059672.2	Q7KZI7-4	full length	-	baculovirus in insect cells	N-terminal GST- tag
MARK3	MARK3	CHKtide	NP_002367.3	P27448	full length	-	baculovirus in insect cells	N-terminal GST- tag
MARK4	MARK4	CHKtide	NP_113605	Q96L34	full length	-	baculovirus in insect cells	N-terminal GST- tag
MEK1	MAP2K1	ERK(K52R)	NP_002746	Q02750	full length	-	baculovirus in insect cell, activated by RAF1 in vivo	N-terminal His6- tag
MEK2	MAP2K2	ERK(K52R)	NP_109587	P36507	full length	-	baculovirus in insect cells, activated by co- expression with RAF1	C-terminal His6- tag

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MEKK2	MAP3K2	MBP	NM_006609	Q9Y2U5	full length	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
MEKK3	MAP3K3	MBP	NM_002401	Q99759	full length	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
MELK	MELK	ZIptide	NP_055606.1	Q14680	aa 1-340	-	Insect cell	N-terminal GST-tag
MINK/MINK1	MINK1	MBP	NP_056531	Q8N4C8	full catalytic	-	Insect	N-terminal GST
MKK4	MAP2K4	JNK(K55M)	NM_003010	P45985	aa 33-end		baculovirus in Sf9 insect cells	N-terminal His-tag
MKK6	MAP2K6	MBP	NP_002749	P52564	full length	S207E, T211E	E. coli	N-terminal His-tag
MLCK/MYLK	MYLK	ZIptide + Ca-CaM	NP_444253	Q15746	Catalytic (aa 1428-1771)		Insect	N-terminal GST
MLCK2/MYLK2	MYLK2	ZIptide + Ca-CaM	NP_149109	Q9H1R3	full length		Insect	N-terminal GST
MLK1/MAP3K9	MAP3K9	Casein	NP_149132.1	P80192	full catalytic	-	Insect	N-terminal GST
MLK2/MAP3K10	MAP3K10	MBP	NP_002437	Q02779	full catalytic	-	Insect	N-terminal GST
MLK3/MAP3K11	MAP3K11	MBP	NP_002410.1	Q16584	full catalytic	-	Insect	N-terminal GST
MNK1	MKNK1	MBP	GenBank NM_003684	Q9BUB5	aa2-end (deletion aa165-205)	T385D	baculovirus in Sf9 insect cells	N-terminal GST
MNK2	MKNK2	MBP	NP_060042.2	Q9HBH9	full length	-	Baculovirus infected insect cells	N-terminal GST
MRCKa/CDC42BPA	CDC42BPA	Long S6 Kinase substrate peptide	NP_055641	Q5VT25	aa 1-473	-	Baculovirus infected insect cells	C-terminal 6X-His tag
MRCKb/CDC42BPB	CDC42BPB	Long S6 Kinase substrate peptide	NP_006026.2	Q9Y5S2	aa 1-473	-	Baculovirus infected insect cells	C-terminal 6X-His tag

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MSK1/RPS6KA5	RPS6KA5	Crosstide	NP_004746.2	O75582	full-length	-	Insect	N-terminal GST
MSK2/RPS6KA4	RPS6KA4	Crosstide	NP_003933	O75676	full-length	-	Insect	N-terminal GST
MSSK1/STK23	SRPK3	RS peptide	NP_055185	Q9UPE1	full-length	-	Insect	N-terminal GST
MST1/STK4	STK4	Axltide	NP_006273	Q13043	full-length	-	Insect	N-terminal GST
MST2/STK3	STK3	MBP	NP_006272.2	Q13188	full length	-	Insect	N-terminal GST
MST3/STK24	STK24	MBP	NP_003567	Q9Y6E0	full length	-	Insect	N-terminal GST
MST4	MST4	MBP	NP_057626.2	Q9P289	full-length	-	Insect	N-terminal GST
MUSK	MUSK	MBP	NP_005583.1	O15146	cytoplasmic	-	Insect	N-terminal GST
MYLK3	MYLK3	MYLK3	ZIPtide + Ca-CaM	BC109097	Q32MK0	full-length	Insect	N-terminal GST
MYO3B	MYO3B	MYO3B	MBP	NM_138995	Q8WXR4	Catalytic (1-326)	Insect	N-terminal GST
NEK1	NEK1	MBP	NP_036356	Q96PY6	aa 1-505	-	Insect	N-terminal GST
NEK11	NEK11	MBP	NP_079076	Q8NG66	full-length	-	Baculovirus infected insect cells	N-terminal GST
NEK2	NEK2	MBP	NP_002488	P51955	full-length	-	Insect	C-terminal His6-tagged
NEK3	NEK3	MBP	NP_689933	Q8WUN5	full-length	-	Insect	N-terminal GST
NEK4	NEK4	MBP	NP_003148	P51957	full-length	-	Insect	N-terminal GST
NEK6	NEK6	MBP	NP_055212	Q9HC98	aa 7-313	-	baculovirus insect cell	C-terminal His-tag
NEK7	NEK7	MBP	NP_598001.1	Q8TDX7	full length	-	Insect	N-terminal GST tag
NEK9	NEK9	MBP	NP_149107.2	Q8TD19	Catalytic (aa 347-732)	-	Insect	N-terminal GST tag
NIK/MAP3K14	MAP3K14	MBP	NP_003945.2	Q99558	Catalytic (aa 318-947)	-	Insect	N-terminal GST tag
NLK	NLK	MBP	NP_057315.1	Q9UBE8	full length	-	Insect	N-terminal GST
OSR1/OXSR1	OXSR1	CATCHtide	NP_005100.1	O95747	full length	-	Baculovirus infected insect cells	N-terminal GST

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
P38a/MAPK14	MAPK14	MBP	NP_620581	Q16539	full-length	-	E. coli	N-terminal GST
P38b/MAPK11	MAPK11	MBP	NP_002742	Q15759	full-length	-	Insect	N-terminal His
P38d/MAPK13	MAPK13	MBP	NP_002745	O15264	full-length	-	Insect	N-terminal His
P38g/MAPK12	MAPK12	MBP	NP_002960	P53778	full-length	-	Insect	N-terminal His
p70S6K/RPS6KB1	RPS6KB1	S6K/Rsk2 peptide 2	NP_003152, T412E	P23443	Catalytic (aa 1-421)	-	Insect	N-terminal GST
p70S6Kb/RPS6KB2	RPS6KB2	S6K/Rsk2 peptide 2	NP_003943	Q9UBS0	full length	-	Insect	N-terminal GST
PAK1	PAK1	Long S6 Kinase substrate peptide	NP_002567	Q13153	full length	-	Insect	N-terminal GST
PAK2	PAK2	Long S6 Kinase substrate peptide	NP_002568.2	Q13177	full length	-	Insect	N-terminal GST
PAK3	PAK3	ZIPtide	NP_002569	O75914	full length	-	Insect	N-terminal His6-tag
PAK4	PAK4	MBP	NP_005875	O96013	Catalytic (aa 295-591)	-	Insect	N-terminal GST
PAK5	PAK7	ZIPtide	NP_065074	Q9P286	aa 425-719	-	Baculovirus infected insect cells	N-terminal 6X-His tag
PAK6	PAK6	ZIPtide	NP_064553	Q9NQU5	full-length	-	Insect	C-terminal His
PASK	PASK	ZIPtide	NP_055963	Q96RG2	full catalytic	-	Insect	N-terminal GST
PBK/TOPK	PBK	MBP	NP_060962	Q96KB5	full catalytic	-	Insect	C-terminal His
PDGFRa	PDGFRA	pEY + Mn	NP_006197	Q9DE49	Cytoplasmic (550-1089)		Insect	N-terminal GST
PDGFRb	PDGFRB	pEY + Mn	NP_002600	P09619	Cytoplasmic (558-1106)		Insect	N-terminal His6-tagged

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
PDK1/PDPK1	PDPK1	PDKtide	NP_002604	O15530	full length	-	Insect	N-terminal His6-tag
PHKg1	PHKG1	ZIPtide	NP_006204	Q16816	full length	-	Insect	N-terminal GST-tag
PHKg2	PHKG2	ZIPtide	NP_000285	P15735	full length	-	Insect	N-terminal GST-tag
PIM1	PIM1	S6K/Rsk2 peptide 2	NP_002639	P11309	full length	-	Insect	C-terminal His tagged
PIM2	PIM2	Pim2tide	NP_006866	Q9P1W9	full-length	-	Insect	N-terminal GST
PIM3	PIM3	Pim2tide	GenBank AB114795	Q86V86	aa 2-end	-	Baculovirus in Sf21 insect cells	N-terminal His6-tag
PKA	PRKACA	PKA sub	NP_002721.1	P17612	Catalytic (1-351)	-	E. coli	N-terminal His6-tag
PKAca	KAPCA	Long S6 Kinase substrate peptide	NM_002730	P17612	full-length	-	baculovirus in Sf9 cells	N-terminal GST
PKAcb	KAPCB	Long S6 Kinase substrate peptide	NM_002730	P22694	full-length	-	baculovirus in Sf9 cells	N-terminal GST
PKAcg	KAPCG	Long S6 Kinase substrate peptide	NM_002732	P22612	full-length	-	Insect	N-terminal GST
PKCa	PRKCA	Histone H1 + Lipid Activator	NP_002728	P17252	full length	-	Insect	none
PKCb1	PRKCB1	Histone H1 + Lipid Activator	NP_991100.1	P05771	full length	-	baculovirus in Sf21 insect cells	none
PKCb2	PRKCB2	Histone H1 + Lipid Activator	NP_002729	P05771	full length	-	insect	none

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
PKCd	PRKCD	PKCe Pep + Lipid Activator	NP_006245	Q05655	full length	-	insect	none
PKCepsilon	PRKCE	S25 PKC Peptide	NP_005391.1	Q02156	full-length	-	Insect	none
PKCeta	PRKCH	PKCe Pep + Lipid Activator	NM_006255	P24723	full length	-	baculovirus in Sf9 insect cells	N-terminal GST
PKCg	PRKCG	Histone H1 + Lipid Activator	NP_002730	P05129	-	-	baculovirus in insect cells	none
PKCiota	PRKCI	PKCepsilon Peptide	NP_002731	P41743	full length	-	baculovirus insect cell	N-terminal His-tag
PKCmu/PRKD1	PRKD1	Glycogen Synthase-derived peptide	NP_002733	Q15139	full length	-	Insect	N-terminal GST
PKCnu/PRKD3	PRKD3	Glycogen Synthase-derived peptide	NP_005804	O94806	full-length	-	Insect	N-terminal GST
PKCtheta	PRKCQ	Histone H1 + Lipid Activator	NP_006248	Q04759	full length	P330L	baculovirus in insect cells	C-terminal His6-tag
PKCzeta	PRKCZ	PKCepsilon Peptide	NP_002735	Q05513	full-length	-	Insect	none
PKD2/PRKD2	PRKD2	Glycogen Synthase-derived peptide	NP_057541	Q9BZL6	full-length	-	Insect	N-terminal GST
PKG1a	PRKG1	Kemptide	NM_001098512	Q13976	full length	-	baculovirus in Sf9 cells	N-terminal His6-tag
PKG1b	PRKG1	Kemptide	GenBank NM_006258	P14619	full length	-	baculovirus in Sf21 insect cells	N-terminal His6-tag
PKG2/PRKG2	PRKG2	Kemptide	NP_006250	Q13237	full length	-	Insect	N-terminal GST

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
PKN1/PRK1	PKN1	Glycogen Synthase-derived peptide	NP_998725	Q16512	full length	-	Insect	N-terminal GST
PKN2/PRK2	PKN2	Glycogen Synthase-derived peptide	NP_006247	Q16513	full length	-	Insect	N-terminal GST
PLK1	PLK1	Casein	NP_005021	P53350	full length	-	Insect	C-terminal His6-tag
PLK2	PLK2	Casein	NP_006613	Q9NYY3	full length	-	Insect	N-terminal GST-His6 tag
PLK3	PLK3	Casein	NP_004064	Q9H4B4	Catalytic (58-340)	-	Insect	N-terminal GST
PRKX	PRKX	Kemptide	NP_722560	P51817	full length	-	Insect	N-terminal GST
PYK2	PTK2B	pEY + Mn	NP_004094	Q14289	full-length	-	Insect	N-terminal GST
RAF1	RAF1	MEK1 (K97R)	NP_002871	P04049	full catalytic	-	Insect	N-terminal GST
RET	RET	CHKtide	NP_066124	P07949	cytoplasmic	-	Insect	N-terminal GST
RIPK2	RIPK2	MBP	NP_003812	O43353	aa 1-299	-	Baculovirus infected insect cells	N-terminal 6X-His tag
RIPK5	DSTYK	MBP	NP_056190.1	Q6XUX3	full length	-	Insect	N-terminal GST
ROCK1	ROCK1	Long S6 Kinase substrate peptide	NP_005397	Q13464	aa 1-535	-	Insect	N-terminal GST
ROCK2	ROCK2	Long S6 Kinase substrate peptide	NM_004850	O75116	aa 5-554	-	baculovirus in Sf9 insect cells	N-terminal GST
RON/MST1R	MST1R	Axltide + Mn	NP_002438	Q04912	aa 983-1400	-	Baculovirus infected insect cells	N-terminal GST
ROS/ROS1	ROS1	IGF-1Rtide	NP_002935	P08922	cytoplasmic	-	Insect	N-terminal GST

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
RSK1	RPS6KA1	Glycogen Synthase-derived peptide	NP_002944	Q15418	full length	-	Insect	N-terminal His6-tag
RSK2	RPS6KA3	Glycogen Synthase-derived peptide	NP_004577	P51812	full length	-	baculovirus insect cell	C-terminal His-tag
RSK3	RPS6KA2	Glycogen Synthase-derived peptide	NP_066958	Q15349	full length	-	Insect	N-terminal His6-tag
RSK4	RPS6KA6	Long S6 Kinase substrate peptide	NP_055311	Q9UK32	full-length	-	Insect	N-terminal GST
SGK1	SGK1	Crosstide	NP_005618, S589D	O00141	Catalytic (60-431)	S422D	Insect	N-terminal GST
SGK2	SGK2	Crosstide		Q9HBY8	full length (Met1-Cys367)	-	baculovirus expression system	GST-tag
SGK3/SGKL	SGK3	Crosstide	NP_037389, S487D	Q96BR1	Catalytic (87-496)	-	Insect	N-terminal GST-tag
SIK2	SIK2	Kemptide	NP_056006.1	Q9H0K1	full length	-	Insect	N-terminal GST-tag
SLK/STK2	SLK	Histone H3	NP_055535.1	Q9H2G2	full length	-	Insect	N-terminal GST-tag
SNARK/NUAK2	NUAK2	MBP	NM_030952	Q9H093	aa M1-T628	-	baculovirus in Sf9 insect cells	N-terminally fused to GST-His6
SRMS	SRMS	pEY + Mn	NP_543013	Q9H3Y6	full length	-	Insect	N-terminal GST
SRPK1	SRPK1	RS peptide	NP_003128	Q96SB4	full length	-	Insect	N-terminal His-tag
SRPK2	SRPK2	RS peptide	NP_872633	P78362	full length	-	Insect	N-terminal GST-tag
STK16	STK16	MBP	NP_003682	O75716	full length	-	Insect	N-terminal His-tag

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
STK22D/TSSK1	TSSK1B	CHKtide	NP_114417	Q9BXA7	full length	-	Insect	C-terminal His-tag
STK25/YSK1	STK25	MBP	NP_006365	O00506	full length	-	Insect	N-terminal GST
STK33	STK33	MBP	NP_112168	Q9BYT3	full length	-	Insect	N-terminal His-tag
STK38/NDR1	STK38/NDR1	STK38	Modified PKA Substrate	NM_007271	Q15208	full-length	Insect	N-terminal GST
STK39/STLK3	STK39	CATCHtide	NP_037365.2	Q9UEW8	full length	-	Insect	N-terminal GST
SYK	SYK	pEY	NP_003168	P43405	full-length	-	Insect	N-terminal GST
TAK1	MAP3K7/MA P3K7IP1	Casein	NP_663306, NP_006107	MAP3K7:O43 318; TAB1:Q15750	full-length MAP3K7; aa 437-504 MAP3K7IP1	-	Baculovirus infected insect cells	N-terminal 6X-His tag
TAOK1	TAOK1	MBP	NM_020791	Q7L7X3	aa1-314	-	baculovirus in Sf9 insect cells	N-terminal GST
TAOK2	TAOK2	MBP	NP_004774	Q9UL54	full catalytic	-	Insect	N-terminal GST
TAOK3/JIK	TAOK3	MBP	NP_057365	Q9H2K8	full-length	-	Insect	N-terminal GST
TBK1	TBK1	CK1tide	NP_037386	Q9UHD2	full-length	-	Insect	N-terminal GST
TEC	TEC	pEY + Mn	NP_003206	P42680	full length	-	baculovirus insect cell	C-terminal His-tag
TGFBR2	TGFBR2	MBP	NM_003242	P37173	190-end	-	baculovirus in Sf9 insect cells	N-terminal GST
TIE2/TEK	TEK	pEY + Mn	NP_000450	Q02763	Cytoplasmic (817-1101)	-	Insect	N-terminal GST- tag
TLK2	TLK2	TLK2	Casein	NM_006852	Q86UE8	Catalytic (388-end)	Insect	N-terminal GST
TRKA	NTRK1	pEY + Mn	NP_002520	P04629	Cytoplasmic (441-796)	-	insect	C-terminal His-tag
TRKB	NTRK2	pEY + Mn	NP_006171	Q16620	Cytoplasmic (526-838)	-	Insect	C-terminal His-tag
TRKC	NTRK3	pEY	NP_002521.2	Q16288	catalytic domain (aa 510-825)	-	baculovirus insect cell	C-terminal His-tag
TSSK2	TSSK2	CHKtide	NP_443732	Q96PF2	full length	-	Insect	N-terminal His6- tag

RBC Enzyme Name	HUGO symbol	Substrate	Genbank Accession #	Protein Accession #	Clone	Mutation	Expression	Tag
TTK	TTK	MBP	NP_003309	P33981	full-length	-	Insect	N-terminal
TXK	TXK	ABLtide	NP_003319.2	P42681	full length	-	Insect	N-terminal GST-tag
TYK1/LTK	LTK	ABLtide	NP_002335.2	P29376	Cytoplasmic (450-864)	-	Insect	N-terminal GST-tag
TYK2	TYK2	AXLtide	NP_003322.2	P29597	aa 833-1187	-	Insect	N-terminal GST
TYRO3/SKY	TYRO3	pEY + Mn	NP_006284	Q06418	Cytoplasmic (451-890)	-	Insect	N-terminal GST-tag
ULK1	ULK1	MBP	BC111603	O75385	aa 1-649	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
ULK2	ULK2	MBP	NM_014683	Q8IYT8	aa 1-631	-	baculovirus in Sf9 insect cells	N-terminal GST-tag
ULK3	ULK3	ULK3	Casein	BC157884	Q6PHR2	full-length	Insect	N-terminal His6-tag
VRK1	VRK1	Casein	NM_003384	Q99986	full length, Met1-Lys396	-	Sf9 cells	GST-HIS fusion
WEE1	WEE1	MBP	NP_003381.1	P30291	full-length	-	Insect	N-terminal
WNK2	WNK2	MBP	NP_006639.3	Q9Y3S1	Catalytic (166-489)	-	Insect	N-terminal GST
WNK3	WNK3	MBP	NP_065973	Q9BYP7	Catalytic (1-434)	-	Insect	N-terminal His6-tag
YES/YES1	YES1	pEY	NP_005424	P07947	full length	-	Insect	C-terminal His-tag
ZAK/MLTK	ZAK	MBP	NP_598407.1	Q9NYL2	full length	-	Insect	N-terminal GST
ZAP70	ZAP70	pEY	NP_001070	P43403	full length	-	Insect	C-terminal His6-tag
ZIPK/DAPK3	DAPK3	ZIPtide	NP_001339	O43293	full-length	-	Insect	N-terminal GST

Supplementary Table 4. A ranked table of kinases sorted by Selectivity score, the fraction of all tested inhibitors that inhibited the catalytic activity of the test kinase by >50%.

Kinase	Selectivity Score
COT1/MAP3K8	0.000
CTK MATK	0.000
DYRK4	0.000
GRK2	0.000
GRK3	0.000
HIPK1	0.000
JNK3	0.000
MAPKAPK3	0.000
NEK6	0.000
NEK7	0.000
P38d/MAPK13	0.000
P38g	0.000
VRK1	0.000
WNK3	0.000
ALK2/ACVR1	0.006
CAMK1b	0.006
CAMK4	0.006
DMPK	0.006
GRK5	0.006
NEK2	0.006
NEK3	0.006
OSR1/OXSR1	0.006
PLK2	0.006
RON/MST1R	0.006
SGK3/SGKL	0.006
STK39/STLK3	0.006
WNK2	0.006
MRCKa/CDC42BPA	0.006
AKT2	0.011
ALK4/ACVR1B	0.011
CDK7/cyclin H	0.011
DCAMKL2	0.011
ERK1	0.011
ERK2 MAPK1	0.011
HIPK4	0.011
IKKa/CHUK	0.011
JNK1	0.011
MAPKAPK2	0.011
MRCKb/CDC42BPB	0.011
NEK11	0.011
PKCzeta	0.011
SRPK1	0.011
TSSK2	0.011
WEE1	0.011
ZAP70	0.011
AKT1	0.011
ALK5/TGFBR1	0.011
CAMK1a	0.011
MAPKAPK5/PRAK	0.011
NIK/MAP3K14	0.011
ALK1/ACVRL1	0.017
BRAF	0.017
c-MET	0.017
FGFR4	0.017

Kinase	Selectivity Score
GRK4	0.017
HIPK2	0.017
HIPK3	0.017
IKKb/IKBKB	0.017
PKCiota	0.017
PAK6	0.017
CK1g1	0.022
MEK1	0.022
MKK6	0.022
MSSK1/STK23	0.022
p70S6Kb/RPS6KB2	0.022
PAK4	0.022
SRMS	0.022
TEC	0.022
AKT3	0.023
CAMK1g	0.023
DAPK2	0.023
PBK/TOPK	0.023
TIE2/TEK	0.023
SRPK2	0.023
EPHB3	0.023
ASK1/MAP3K5	0.028
EPHA8	0.028
NEK9	0.028
PAK2	0.028
PAK3	0.028
RIPK5	0.028
TGFBR2	0.028
TTK	0.028
ZIPK/DAPK3	0.028
CK1g2	0.028
DYRK3	0.028
CAMK1d	0.028
PKAcg	0.031
EPHA3	0.034
EPHA5	0.034
EPHA7	0.034
GRK6	0.034
GRK7	0.034
MEK2	0.034
P38b/MAPK11	0.034
PAK5	0.034
PIM2	0.034
PKCg	0.034
PKG1b	0.034
PKN2/PRK2	0.034
PLK1	0.034
STK25/YSK1	0.034
PKA	0.034
SGK2	0.034
CK1g3	0.039
EPHA1	0.039
IGF1R	0.039
NEK4	0.039

Kinase	Selectivity Score
PAK1	0.039
PASK	0.039
PLK3	0.039
PRKX	0.039
ARAF	0.040
PDK1/PDPK1	0.040
CK1a1	0.040
STK38/NDR1	0.040
CAMK2b	0.045
DAPK1	0.045
DDR2	0.045
EPHA4	0.045
EPHB2	0.045
PHKg2	0.045
RAF1	0.045
TLK2	0.050
FAK/PTK2	0.051
IR	0.051
PKCtheta	0.051
SGK1	0.051
SNARK/NUAK2	0.051
NEK1	0.051
PKG1a	0.051
TAOK2/TAO1	0.051
ZAK/MLTK	0.051
CK2a	0.051
EPHB4	0.052
CAMK2g	0.056
CSK	0.056
ITK	0.056
ROCK1	0.056
TYRO3 SKY	0.056
ULK2	0.056
EPHB1	0.056
FES/FPS	0.056
IRR/INSRR	0.056
TAOK1	0.056
TAOK3/JIK	0.056
CDK4/cyclin D1	0.062
CLK3	0.062
DYRK2	0.062
EPHA2	0.062
FRK/PTK5	0.062
JAK1	0.062
MNK1	0.062
MSK1/RPS6KA5	0.062
PKCb1	0.062
JNK2	0.062
P38a/MAPK14	0.062
CK2a2	0.067
CDK4/cyclin D3	0.067
FGFR2	0.067
IKKe/IKBKE	0.067
IRAK4	0.067

Kinase	Selectivity Score
MEKK2	0.067
PKCb2	0.067
PKG2/PRKG2	0.067
CAMKK1	0.068
CDK1/cyclin A	0.068
MST4	0.068
PKCepsilon	0.068
PKCa	0.068
IRAK1	0.073
MEKK3	0.073
PYK2	0.073
SYK	0.073
ALK	0.073
DYRK1/DYRK1A	0.073
ERBB4/HER4	0.073
MARK3	0.073
NLK	0.073
CLK1	0.074
AXL	0.079
CAMK2a	0.079
CAMK2d	0.079
CDK3/cyclin E	0.079
c-MER	0.079
ERBB2/HER2	0.079
FGFR3	0.079
Haspin	0.079
MLK2/MAP3K10	0.079
MUSK	0.079
PKCeta	0.079
ROCK2	0.079
STK16	0.079
ULK1	0.079
MSK2/RPS6KA4	0.079
MYO3b	0.080
ULK3	0.080
CAMKK2	0.084
CDK9/cyclin T1	0.084
DYRK1B	0.084
JAK2	0.084
LKB1	0.084
MARK1	0.084
PKCmu/PRKD1	0.084
TYK1/LTK	0.084
STK22D/TSSK1	0.085
FER	0.090
FGFR1	0.090
FLT1/VEGFR1	0.090
LIMK1	0.090
MARK2/PAR-1Ba	0.090
MST3/STK24	0.090
STK33	0.090
PKD2/PRKD2	0.090
TAK1	0.090
TBK1	0.090

Kinase	Selectivity Score
BMX/ETK	0.096
MLCK/MYLK	0.096
PKCd	0.096
ROS/ROS1	0.096
SIK2	0.096
CHK1	0.096
p70S6K/RPS6KB1	0.096
CDK6/cyclin D1	0.101
LYN B	0.101
MNK2	0.101
DRAK1/STK17A	0.107
PIM1	0.107
SLK/STK2	0.107
TXK	0.107
BRSK2	0.112
EGFR	0.112
MARK4	0.114
ABL1	0.118
Aurora C	0.118
CDK9 cyclin K	0.118
CK1d	0.118
CK1epsilon	0.118
JAK3	0.118
KDR/VEGFR2	0.118
PIM3	0.118
PKCnu/PRKD3	0.118
PKN1/PRK1	0.119
BLK	0.124
BRK	0.124
CDK1/cyclin B	0.124
PDGFRa	0.124
TRKA	0.124
HCK	0.124
BTK	0.129
RIPK2	0.129
BRSK1	0.130
CDK6/cyclin D3	0.130
CLK2	0.135
MELK	0.135
MLCK2/MYLK2	0.135
ABL2/ARG	0.140
Aurora A	0.140
CDK2/cyclin A	0.140
CDK2/cyclin E	0.140
CDK5/p25	0.140
c-SRC	0.140
MINK/MINK1	0.140
PHKg1	0.140
CDK5/p35	0.146
GCK MAP4K2	0.146
LRRK2	0.146
RSK2	0.146
RSK1	0.147
FYN	0.152

Kinase	Selectivity Score
MST2/STK3	0.153
CHK2	0.157
GSK3b	0.157
TYK2	0.157
CLK4	0.163
FLT4/VEGFR3	0.163
PDGFRb	0.164
GSK3a	0.169
LCK	0.169
LYN	0.174
MST1/STK4	0.174
RSK4	0.174
Aurora B	0.180
EPHA6	0.180
ACK1	0.191
FGR	0.191
RSK3	0.191
TRKB	0.191
LOK/STK10	0.198
FMS	0.202
MLK1/MAP3K9	0.202
MLK3/MAP3K11	0.202
c-Kit	0.208
YES/YES1	0.242
ARK5/NUAK1	0.249
RET	0.253
KHS MAP4K5	0.254
HGK MAP4K4	0.264
TRKC	0.271
FLT3	0.410

Supplementary Table 5. A ranked table of compounds sorted by Gini score.

CAS #	Inhibitor name	Gini score	CAS #	Inhibitor name	Gini score
62996-74-1	Staurosporine, Streptomyces sp.	0.20	404828-08-6	GSK-3 Inhibitor XIII	0.57
97161-97-2	K-252a, Nocardiosis sp.	0.29	15966-93-5	VEGF Receptor 2 Kinase Inhibitor I	0.57
135897-06-2	SB 218078	0.36	371935-74-9	PI-103	0.57
443798-55-8	Cdk1/2 Inhibitor III	0.37	546102-60-7	Cdk4 Inhibitor	0.57
608512-97-6	PKR Inhibitor	0.44	40254-90-8	Cdk1/5 Inhibitor	0.57
854171-35-0	Indirubin Derivative E804	0.48	496864-16-5	Aloisine A, RP107	0.57
136194-77-9	Gö 6976	0.49	740841-15-0	GSK-3 Inhibitor X	0.57
856436-16-3	JAK3 Inhibitor VI	0.49	507475-17-4	IKK-2 Inhibitor IV	0.58
326914-10-7	SU11652	0.50	227449-73-2	Syk Inhibitor II	0.58
557795-19-4	Sunitinib	0.52	265312-55-8	Cdk4 Inhibitor III	0.58
120685-11-2	Staurosporine, N-benzoyl-	0.52	129-56-6	JNK Inhibitor II	0.58
244148-46-7	Isogranulatimide	0.52	667463-62-9	GSK-3 Inhibitor IX	0.58
146535-11-7	AG 1296	0.53	19545-26-7	Wortmannin	0.59
331253-86-2	PDK1/Akt/Flt Dual Pathway Inhibitor	0.54	249762-74-1	PDGF Receptor Tyrosine Kinase Inhibitor II	0.59
457081-03-7	JAK Inhibitor I	0.54	167869-21-8	PD 98059	0.59
622387-85-3	Syk Inhibitor	0.54	288144-20-7	VEGF Receptor 2 Kinase Inhibitor II	0.59
5334-30-5	PP3	0.55	114719-57-2	Fascaplysin, Synthetic	0.59
444723-13-1	Cdk2 Inhibitor IV, NU6140	0.56	443797-96-4	Aurora Kinase/Cdk Inhibitor	0.59
216661-57-3	VEGF Receptor 2 Kinase Inhibitor IV	0.56	133053-19-7	Gö 6983	0.59
160807-49-8	Indirubin-3'-monoxime	0.56	175178-82-2	AG 1478	0.60
866405-64-3	AMPK Inhibitor, Compound C	0.56	934358-00-6	Casein Kinase II Inhibitor III, TBCA	0.60

CAS #	Inhibitor name	Gini score	CAS #	Inhibitor name	Gini score
269390-69-4	VEGF Receptor Tyrosine Kinase Inhibitor II	0.60	219138-24-6	p38 MAP Kinase Inhibitor	0.62
171179-06-9	PD 158780	0.60	601514-19-6	GSK3b Inhibitor XII, TWS119	0.62
133052-90-1	Bisindolylmaleimide I	0.60	145915-60-2	PKCbII/EGFR Inhibitor	0.62
71897-07-9	AG 1295	0.60	522629-08-9	MNK1 Inhibitor	0.63
852547-30-9	PKR Inhibitor, Negative Control	0.60	648449-76-7	PI 3-Kg Inhibitor II	0.63
216163-53-0	PD 174265	0.60	516480-79-8	Chk2 Inhibitor II	0.63
204005-46-9	VEGF Receptor 2 Kinase Inhibitor III	0.60	626604-39-5	GSK-3b Inhibitor XI	0.63
212779-48-1	Compound 52	0.60	658084-23-2	Met Kinase Inhibitor	0.63
380843-75-4	Bosutinib	0.61	286370-15-8	VEGF Receptor Tyrosine Kinase Inhibitor III, KRN633	0.63
496864-15-4	Aloisine, RP106	0.61	211555-04-3	JAK3 Inhibitor II	0.63
141992-47-4	Cdk4 Inhibitor II, NSC 625987	0.61	103745-39-7	HA 1077, Dihydrochloride Fasudil	0.63
405169-16-6	Dovitinib	0.61	190654-01-4	Cdk1 Inhibitor, CGP74514A	0.63
3895-92-9	Chelerythrine Chloride	0.61	54642-23-8	JNK Inhibitor, Negative Control	0.63
220749-41-7	Cdk1 Inhibitor	0.61	581098-48-8	p38 MAP Kinase Inhibitor III	0.63
852527-97-0	Alsterpaullone, 2-Cyanoethyl	0.61	666837-93-0	SU9516	0.64
146986-50-7	ROCK Inhibitor, Y-27632	0.61	345616-52-6	ERK Inhibitor III	0.64
144978-82-5	AG 112	0.61	778270-11-4	Bcr-abl Inhibitor	0.64
871307-18-5	Tpl2 Kinase Inhibitor	0.61	70563-58-5	Herbimycin A, Streptomyces sp.	0.64
205254-94-0	PDGF Receptor Tyrosine Kinase Inhibitor III	0.62	34823-86-4	GTP-14564	0.64
896138-40-2	Flt-3 Inhibitor II	0.62	189232-42-6	Bohemine	0.64
220792-57-4	Aminopurvalanol A	0.62	648450-29-7	PI 3-Kg Inhibitor	0.64

CAS #	Inhibitor name	Gini score	CAS #	Inhibitor name	Gini score
2826-26-8	AG 9	0.64	154447-36-6	LY 294002	0.68
58753-54-1	JAK3 Inhibitor IV	0.65	171745-13-4	Compound 56	0.68
237430-03-4	Alsterpaullone	0.65	681281-88-9	Akt Inhibitor IV	0.68
199986-75-9	Cdk2 Inhibitor III	0.65	301836-43-1	Casein Kinase I Inhibitor, D4476	0.68
330161-87-0	SU6656	0.65	639089-54-6	Tozasertib	0.68
852045-46-6	Flt-3 Inhibitor III	0.65	139298-40-1	KN-93	0.69
127243-85-0	H-89, Dihydrochloride	0.65	396129-53-6	TGF- β RI Kinase Inhibitor	0.69
119139-23-0	Bisindolylmaleimide IV	0.65	327036-89-5	GSK-3 β Inhibitor I	0.69
627518-40-5	PDGF Receptor Tyrosine Kinase Inhibitor IV	0.66	212844-53-6	Purvalanol A	0.69
152121-53-4	PD 169316	0.66	257879-35-9	PKC β Inhibitor	0.69
1485-00-3	Syk Inhibitor III	0.66	300801-52-9	Cdc2-Like Kinase Inhibitor, TG003	0.69
186611-52-9	IC261	0.66	154447-38-8	LY 303511- Negative control	0.69
133550-30-8	AG 490	0.66	184475-35-2	Gefitinib	0.69
879127-16-9	Aurora Kinase Inhibitor III	0.66	19542-67-7	BAY 11-7082	0.69
221244-14-0	PP1 Analog II, 1NM-PP1	0.67	366017-09-6	Mubritinib	0.70
196868-63-0	IGF-1R Inhibitor II	0.67	509093-47-4	IRAK-1/4 Inhibitor	0.70
356559-13-2	TGF- β RI Inhibitor III	0.67	186692-46-6	Roscovitine	0.70
174709-30-9	BPIQ-I	0.67	865362-74-9	ERK Inhibitor II, FR180204	0.70
347155-76-4	PDGF RTK Inhibitor	0.67	127191-97-3	KN-62	0.70
301305-73-7	Flt-3 Inhibitor	0.67	183319-69-9	Erlotinib	0.70
345987-15-7	JNK Inhibitor V	0.67	142273-20-9	Kenpaullone	0.70

CAS #	Inhibitor name	Gini score	CAS #	Inhibitor name	Gini score
487021-52-3	GSK-3b Inhibitor VIII	0.70	913844-45-8	Rho Kinase Inhibitor IV	0.74
444731-52-6	Pazopanib	0.71	152121-47-6	SB 203580	0.74
7272-84-6	Rho Kinase Inhibitor III, Rockout	0.71	305350-87-2	MEK1/2 Inhibitor	0.74
318480-82-9	SC-68376	0.71	623163-52-0	MEK Inhibitor II	0.74
41179-33-3	MK2a Inhibitor	0.71	587871-26-9	ATM Kinase Inhibitor	0.74
65678-07-1	AG 1024	0.71	120166-69-0	Diacylglycerol Kinase Inhibitor II	0.74
478482-75-6	GSK-3b Inhibitor II	0.71	302962-49-8	Dasatinib	0.74
52029-86-4	STO-609	0.72	226717-28-8	AGL 2043	0.75
53123-88-9	Rapamycin	0.72	172747-50-1	SB 202474, Negative control for p38 MAPK	0.75
5812-07-7	DMBI	0.72	905973-89-9	ATM/ATR Kinase Inhibitor	0.75
784211-09-2	Cdk/Crk Inhibitor	0.72	443913-73-3	Vandetanib	0.75
404009-46-7	DNA-PK Inhibitor V	0.72	870483-87-7	cFMS Receptor Tyrosine Kinase Inhibitor	0.75
745833-23-2	VX-702	0.73	35943-35-2	Akt Inhibitor V, Triciribine	0.75
894804-07-0	JNK Inhibitor VIII	0.73	312917-14-9	JNK Inhibitor IX	0.75
545380-34-5	NF-kB Activation Inhibitor	0.73	213743-31-8	Lck Inhibitor	0.75
212141-51-0	Vatalanib	0.73	72873-74-6	SKF-86002	0.75
312636-16-1	Sphingosine Kinase Inhibitor	0.73	612847-09-3	Akt Inhibitor VIII, Isozyme-Selective, Akti-1/2	0.75
404009-40-1	DNA-PK Inhibitor III	0.73	151342-35-7	Ro-32-0432	0.76
477600-75-2	Tofacitinib	0.73	152121-30-7	SB 202190	0.76
154447-35-5	DNA-PK Inhibitor II	0.73	220127-57-1	Imatinib	0.77
297744-42-4	MEK Inhibitor I	0.74	925681-41-0	Akt Inhibitor X	0.77

CAS #	Inhibitor name	Gini score
165806-53-1	SB220025	0.77
231277-92-2	Lapatinib	0.77
641571-10-0	Nilotinib	0.78
879127-07-8	EGFR Inhibitor	0.78
179248-59-0	Src Kinase Inhibitor I	0.78
387867-13-2	Tandutinib	0.78
284461-73-0	Sorafenib	0.79
179248-61-4	EGFR/ErbB-2 Inhibitor	0.79
881001-19-0	EGFR/ErbB-2/ErbB-4 Inhibitor	0.79
790299-79-5	Masitinib	0.81